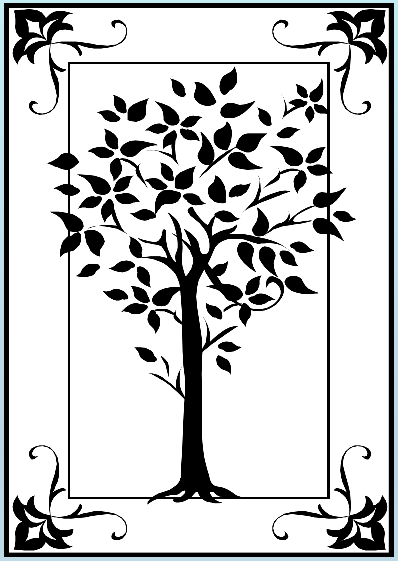
METADATA AND NUMERICAL DATA CAPTURE:
DENSITY (2 component mixture)

Guided Data Capture (GDC)



This tutorial decribes
METADATA AND NUMERICAL DATA CAPTURE:
for **DENSITIES (2 components)**
with the Guided Data Capture (GDC) software.

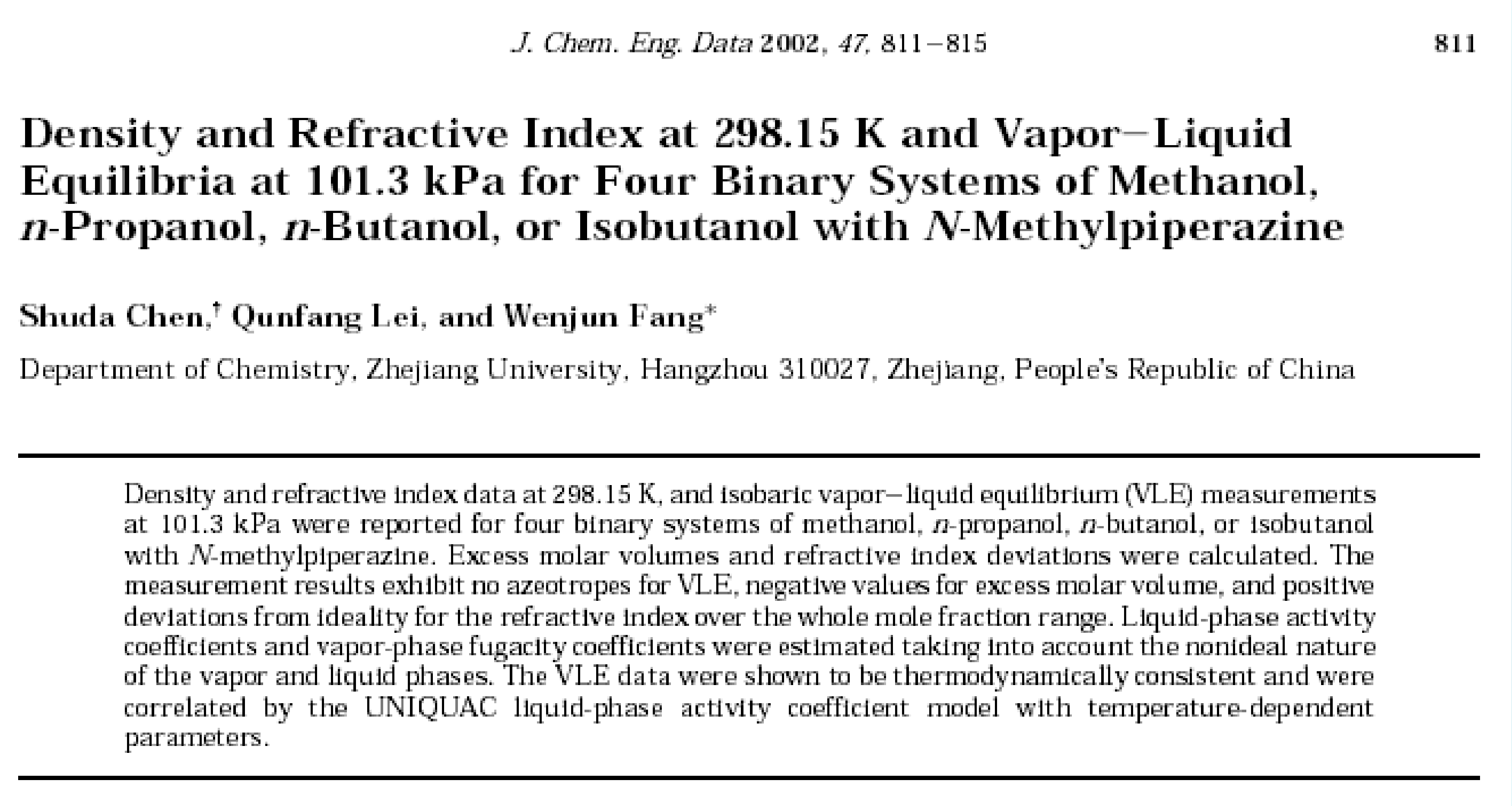
NOTE:

The tutorials proceed sequentially to ease the descriptions. It is not necessary to enter *all* compounds before entering *all* samples, etc.

Compounds, samples, properties, etc., can be added or modified at any time.

However, the hierarchy must be maintained (i.e., a property cannot be entered, if there is no associated sample or compound.)

The experimental data used in this example is from:



J. Chem. Eng. Data 2002, *47,* 811−815 811

Density and Refractive Index at 298.15 K and Vapor−Liquid Equilibria at 101.3 kPa for Four Binary Systems of Methanol, *n*-Propanol, *n*-Butanol, or Isobutanol with *N*-Methylpiperazine

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Density and refractive index data at 298.15 K, and isobaric vapor−liquid equilibrium (VLE) measurements at 101.3 kPa were reported for four binary systems of methanol, *n*-propanol, *n*-butanol, or isobutanol with *N*-methylpiperazine. Excess molar volumes and refractive index deviations were calculated. The measurement results exhibit no azeotropes for VLE, negative values for excess molar volume, and positive deviations from ideality for the refractive index over the whole mole fraction range. Liquid-phase activity coefficients and vapor-phase fugacity coefficients were estimated taking into account the nonideal nature of the vapor and liquid phases. The VLE data were shown to be thermodynamically consistent and were correlated by the UNIQUAC liquid-phase activity coefficient model with temperature-dependent parameters.

Densities (liquid phase) for **(methanol + N-methylpiperazine)** at T = 298.15 K and p = 101.3 kPa

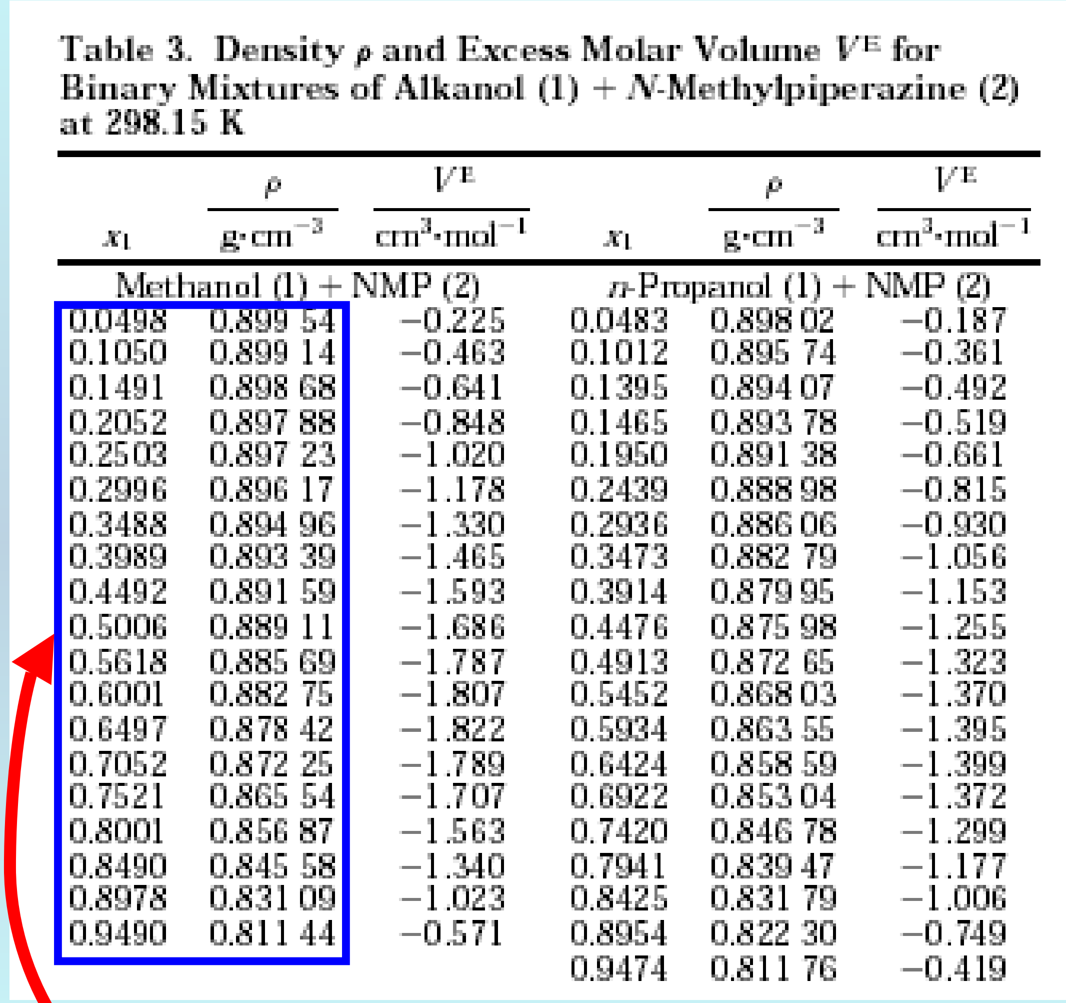
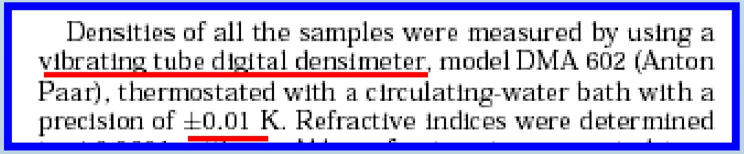


Table 3. Density ρ and Excess Molar Volume V^E for Binary Mixtures of Alkanol (1) + *N*-Methylpiperazine (2) at 298.15 K

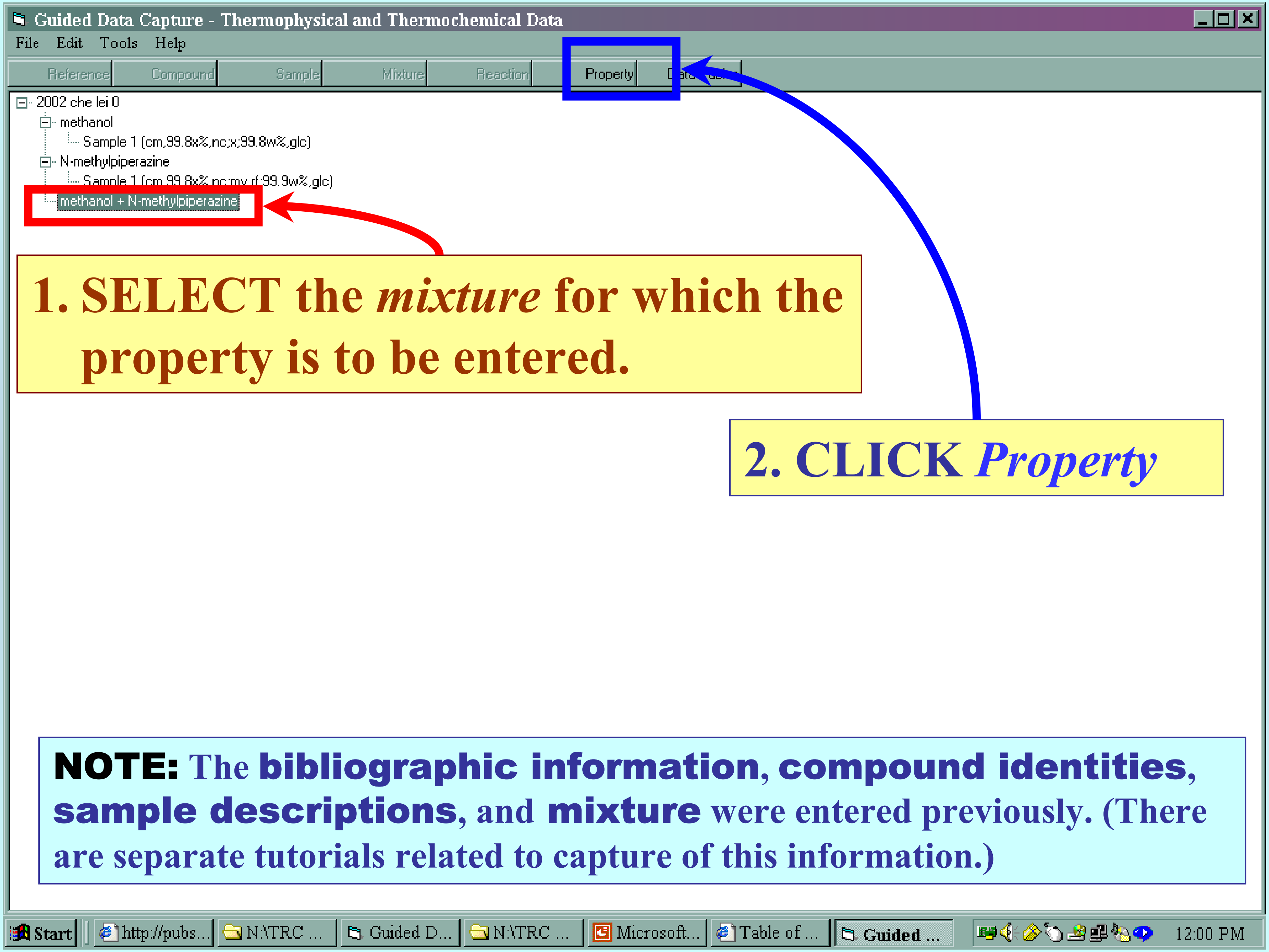
x_1	ρ / $g\cdot cm^{-3}$	V^E / $cm^3\cdot mol^{-1}$	x_1	ρ / $g\cdot cm^{-3}$	V^E / $cm^3\cdot mol^{-1}$
Methanol (1) + NMP (2)			*n*-Propanol (1) + NMP (2)		
0.0498	0.899 54	−0.225	0.0483	0.898 02	−0.187
0.1050	0.899 14	−0.463	0.1012	0.895 74	−0.361
0.1491	0.898 68	−0.641	0.1395	0.894 07	−0.492
0.2052	0.897 88	−0.848	0.1465	0.893 78	−0.519
0.2503	0.897 23	−1.020	0.1950	0.891 38	−0.661
0.2996	0.896 17	−1.178	0.2439	0.888 98	−0.815
0.3488	0.894 96	−1.330	0.2936	0.886 06	−0.930
0.3989	0.893 39	−1.465	0.3473	0.882 79	−1.056
0.4492	0.891 59	−1.593	0.3914	0.879 95	−1.153
0.5006	0.889 11	−1.686	0.4476	0.875 98	−1.255
0.5618	0.885 69	−1.787	0.4913	0.872 65	−1.323
0.6001	0.882 75	−1.807	0.5452	0.868 03	−1.370
0.6497	0.878 42	−1.822	0.5934	0.863 55	−1.395
0.7052	0.872 25	−1.789	0.6424	0.858 59	−1.399
0.7521	0.865 54	−1.707	0.6922	0.853 04	−1.372
0.8001	0.856 87	−1.563	0.7420	0.846 78	−1.299
0.8490	0.845 58	−1.340	0.7941	0.839 47	−1.177
0.8978	0.831 09	−1.023	0.8425	0.831 79	−1.006
0.9490	0.811 44	−0.571	0.8954	0.822 30	−0.749
			0.9474	0.811 76	−0.419

The data set considered here.

Experimental Method:



Densities of all the samples were measured by using a vibrating tube digital densimeter, model DMA 602 (Anton Paar), thermostated with a circulating-water bath with a precision of ±0.01 K. Refractive indices were determined


Guided Data Capture - Thermophysical and Thermochemical Data
File
Edit
Tools
Help
Reference
Compound
Sample
Mixture
Reaction
Property
Start
http://pubs...
N:\TRC ...
Guided D...
N:\TRC ...
Microsoft...
Table of ...
Guided ...
12:00 PM

2002 che lei 0
- methanol
  - Sample 1 (cm,99.8x%,nc;x;99.8w%,glc)
- N-methylpiperazine
  - Sample 1 (cm,99.8x%,nc;mv,rf;99.9w%,glc)
- methanol + N-methylpiperazine

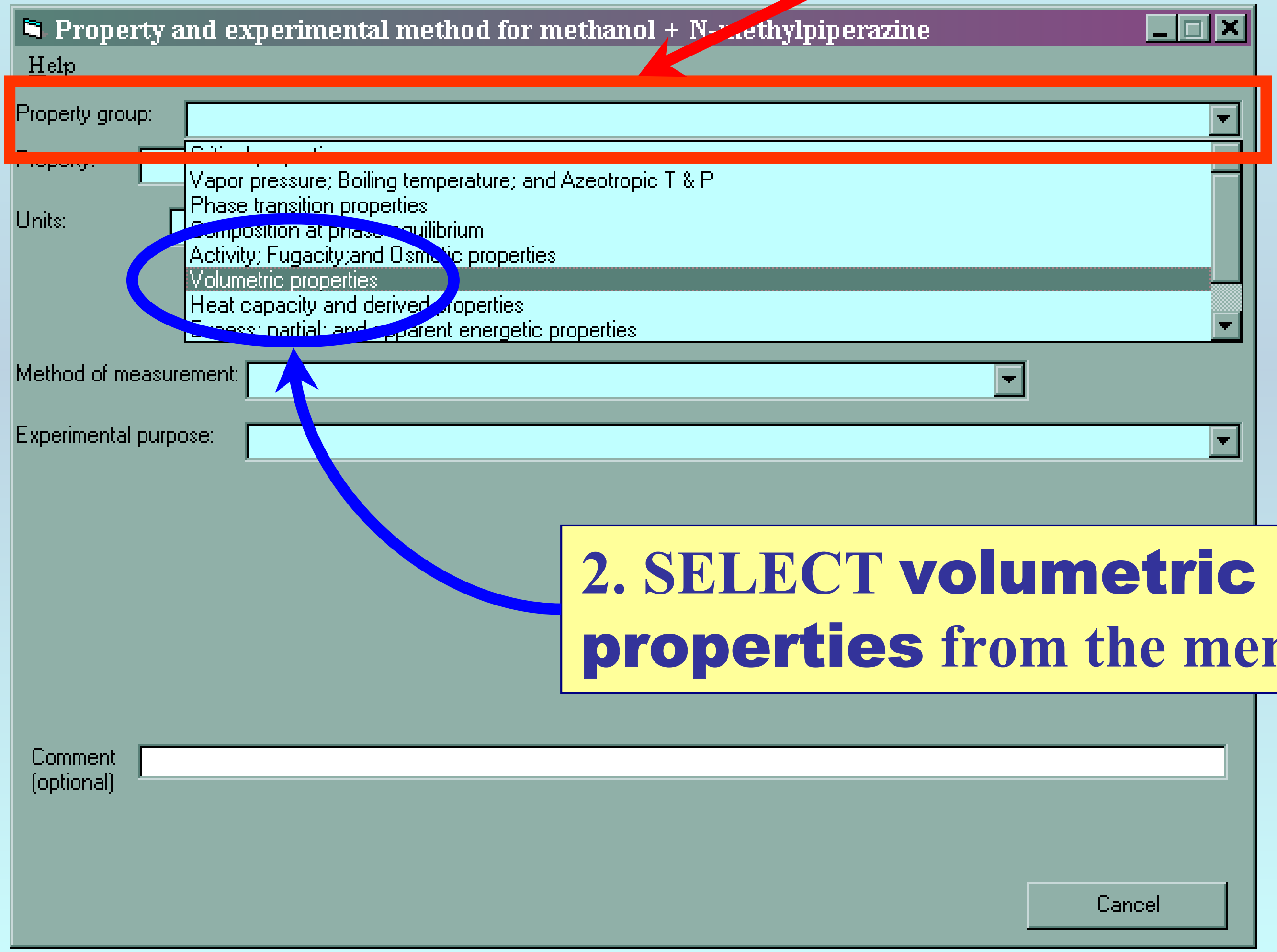
1. **SELECT the *mixture* for which the property is to be entered.**

2. **CLICK *Property***

NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials related to capture of this information.)

Property Group selection

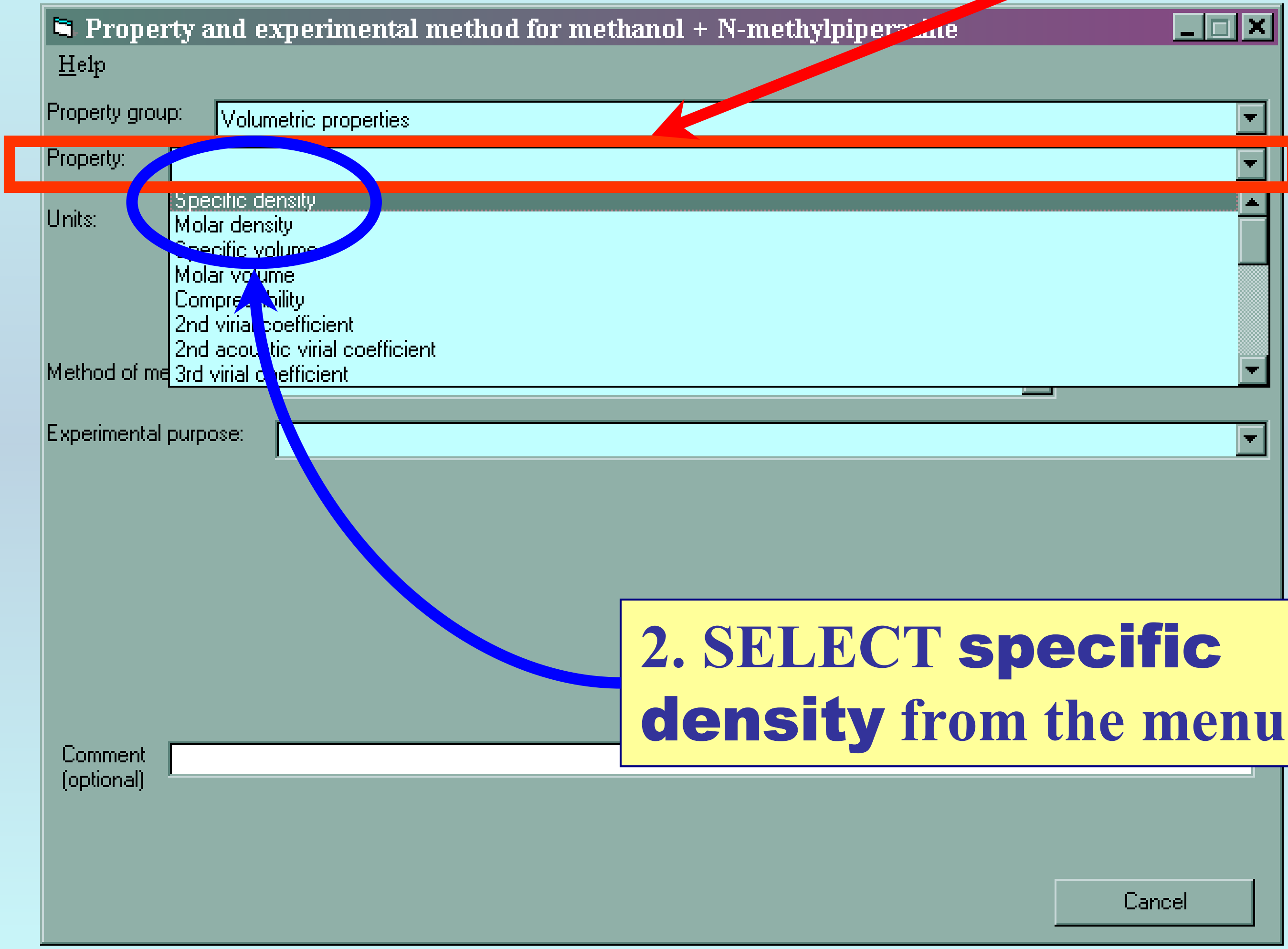
1. CLICK in the **property group** field.


Property and experimental method for methanol + N-methylpiperazine
Help
Property group:
Property:
Units:
Critical properties
Vapor pressure; Boiling temperature; and Azeotropic T & P
Phase transition properties
Composition at phase equilibrium
Activity; Fugacity;and Osmotic properties
Volumetric properties
Heat capacity and derived properties
Excess; partial; and apparent energetic properties
Method of measurement:
Experimental purpose:
Comment
(optional)
Cancel

2. SELECT **volumetric properties** from the menu.

Property selection

1. CLICK in the **property** field.



Property and experimental method for methanol + N-methylpiperazine

Property group: Volumetric properties

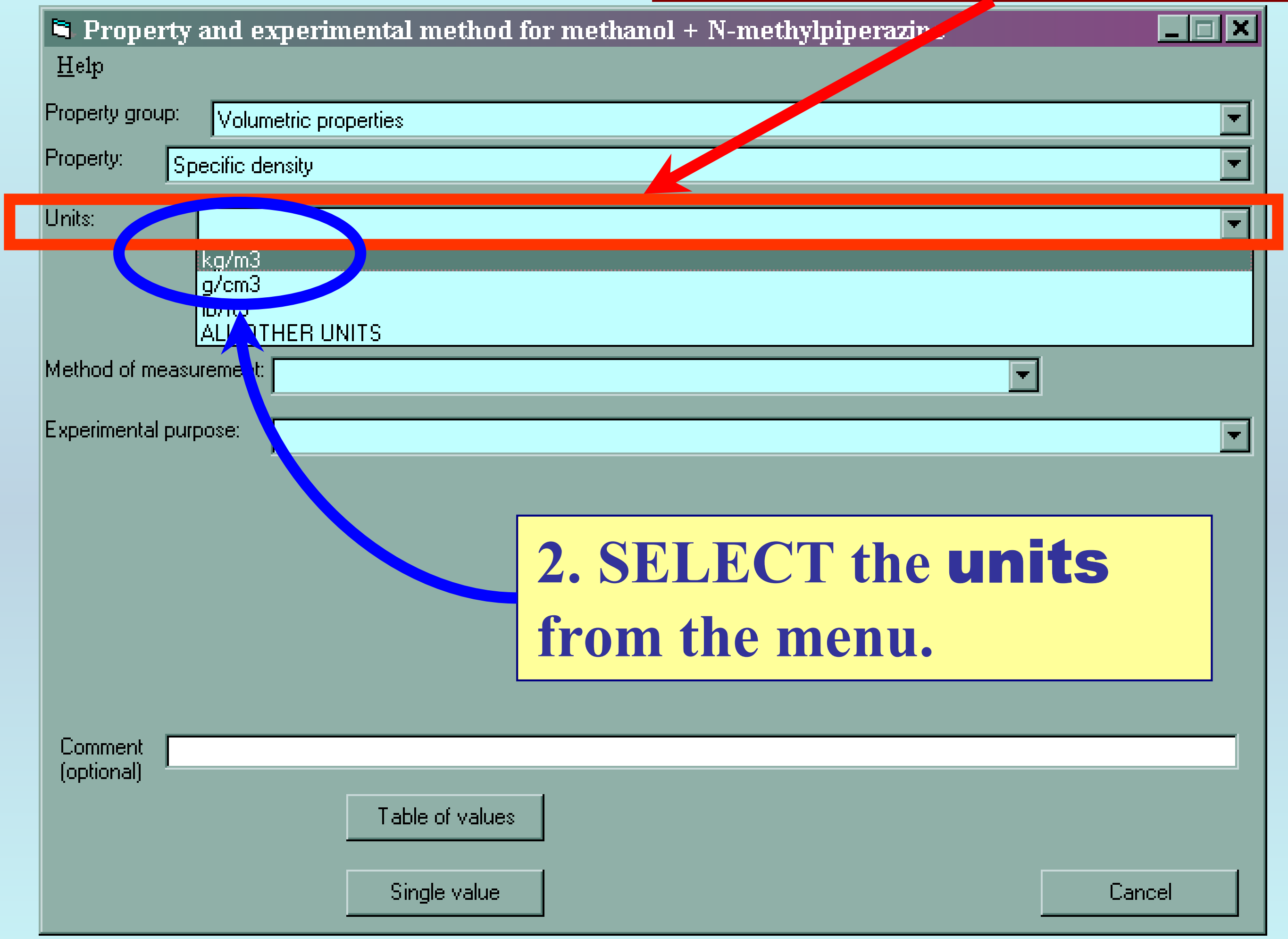
Property:

Help
Specific density
Molar density
Specific volume
Molar volume
Compressibility
2nd virial coefficient
2nd acoustic virial coefficient
3rd virial coefficient
Units:
Method of me
Experimental purpose:
Comment
(optional)
Cancel

2. SELECT **specific density** from the menu.

Units selection

1. CLICK in the units field.


Help
Table of values
Single value
Cancel

Property and experimental method for methanol + N-methylpiperazin

Property group: Volumetric properties

Property: Specific density

Units:

kg/m3
g/cm3
lb/ft3
ALL OTHER UNITS

Method of measurement:

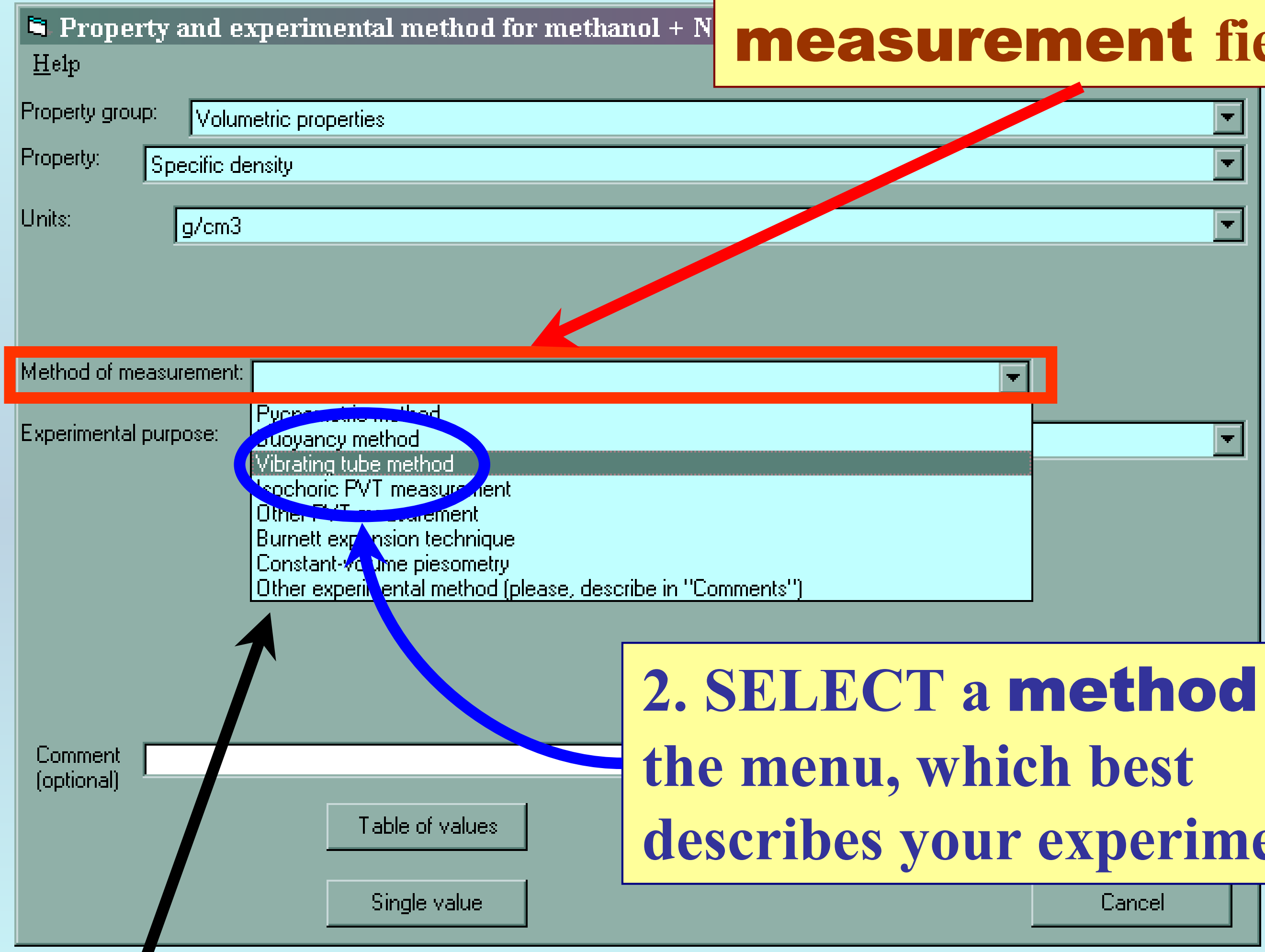
Experimental purpose:

Comment (optional)

2. SELECT the units from the menu.

Method selection

1. CLICK in the **method of measurement** field.


Property and experimental method for methanol + N
Help
Table of values
Single value
Cancel

Property group: Volumetric properties

Property: Specific density

Units: g/cm3

Method of measurement:

Experimental purpose:

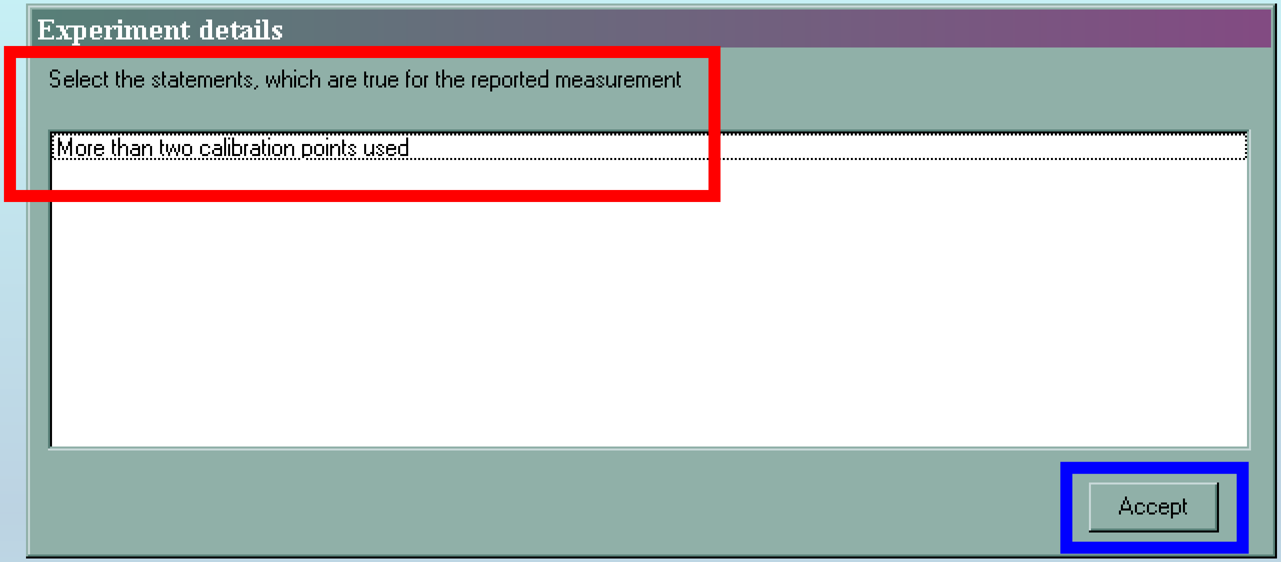
- Pycnometric method
- Buoyancy method
- Vibrating tube method
- Isochoric PVT measurement
- Other PVT measurement
- Burnett expansion technique
- Constant-volume piezometry
- Other experimental method (please, describe in "Comments")

Comment (optional)

2. SELECT a **method** from the menu, which best describes your experiment

Note: *Other* is an option. A one sentence description or a reference is often adequate.

Method detail selection

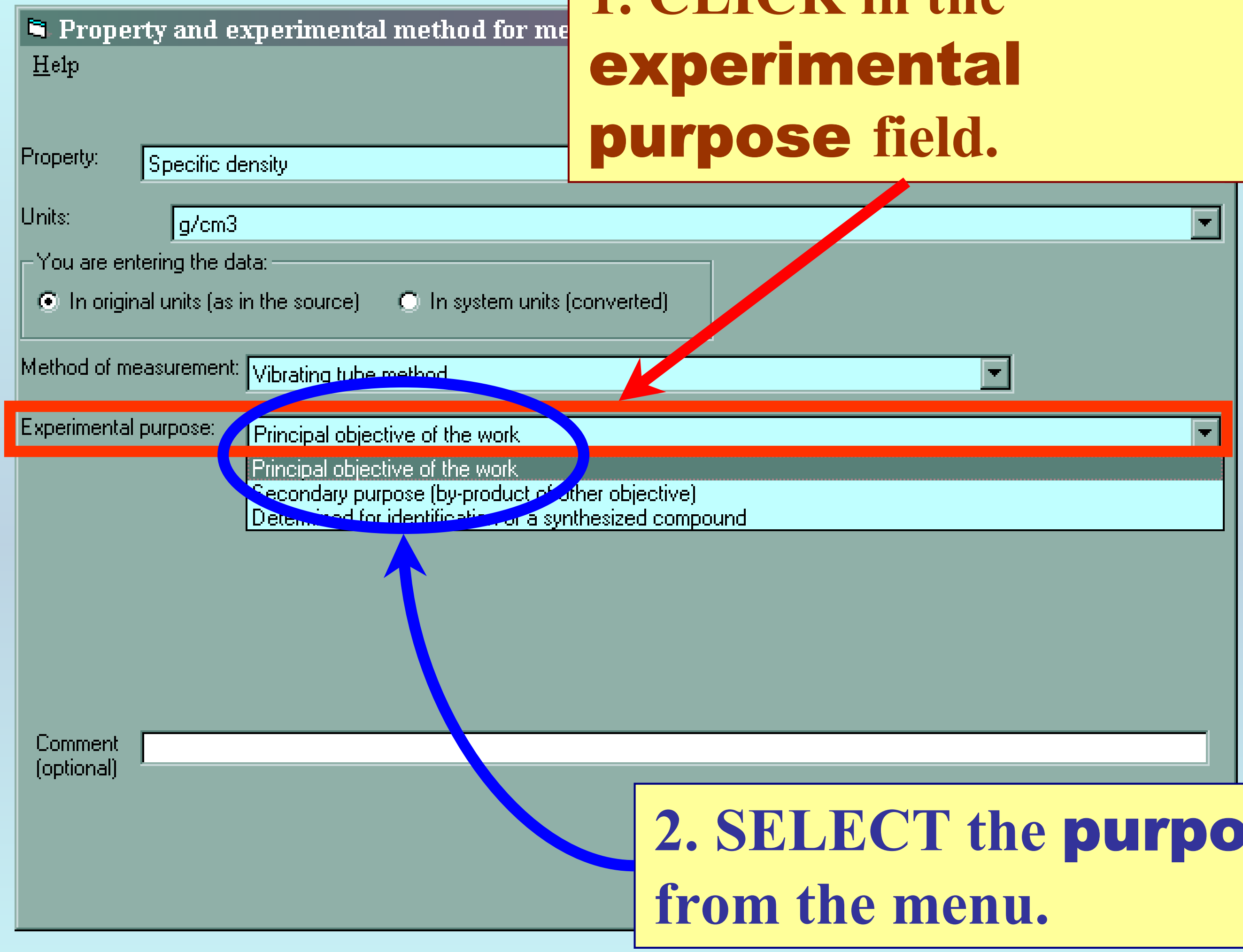

Experiment details

Select the statements, which are true for the reported measurement

More than two calibration points used

Note: **For a few methods, additional details are requested. SELECT those statements that apply, and CLICK *Accept*.**

Experimental purpose selection



Property: Specific density

Units: g/cm3

You are entering the data:

● In original units (as in the source) ○ In system units (converted)

Method of measurement: Vibrating tube method

Experimental purpose: Principal objective of the work

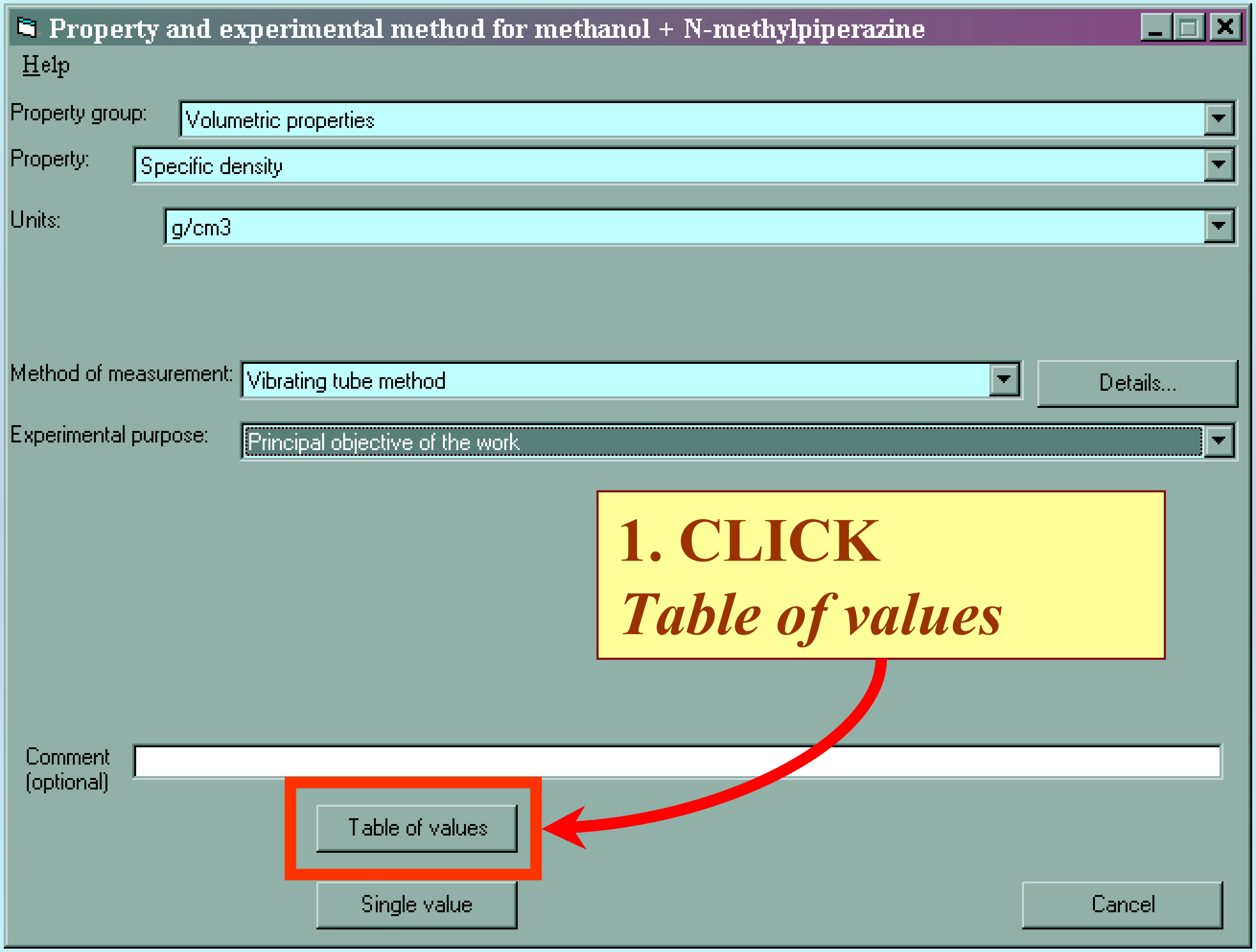
- Principal objective of the work
- Secondary purpose (by-product of other objective)
- Determined for identification of a synthesized compound

Comment (optional)

1. CLICK in the **experimental purpose** field.

2. SELECT the **purpose** from the menu.

Form is complete...



Property and experimental method for methanol + N-methylpiperazine

Property group: Volumetric properties

Property: Specific density

Units: g/cm3

Method of measurement: Vibrating tube method

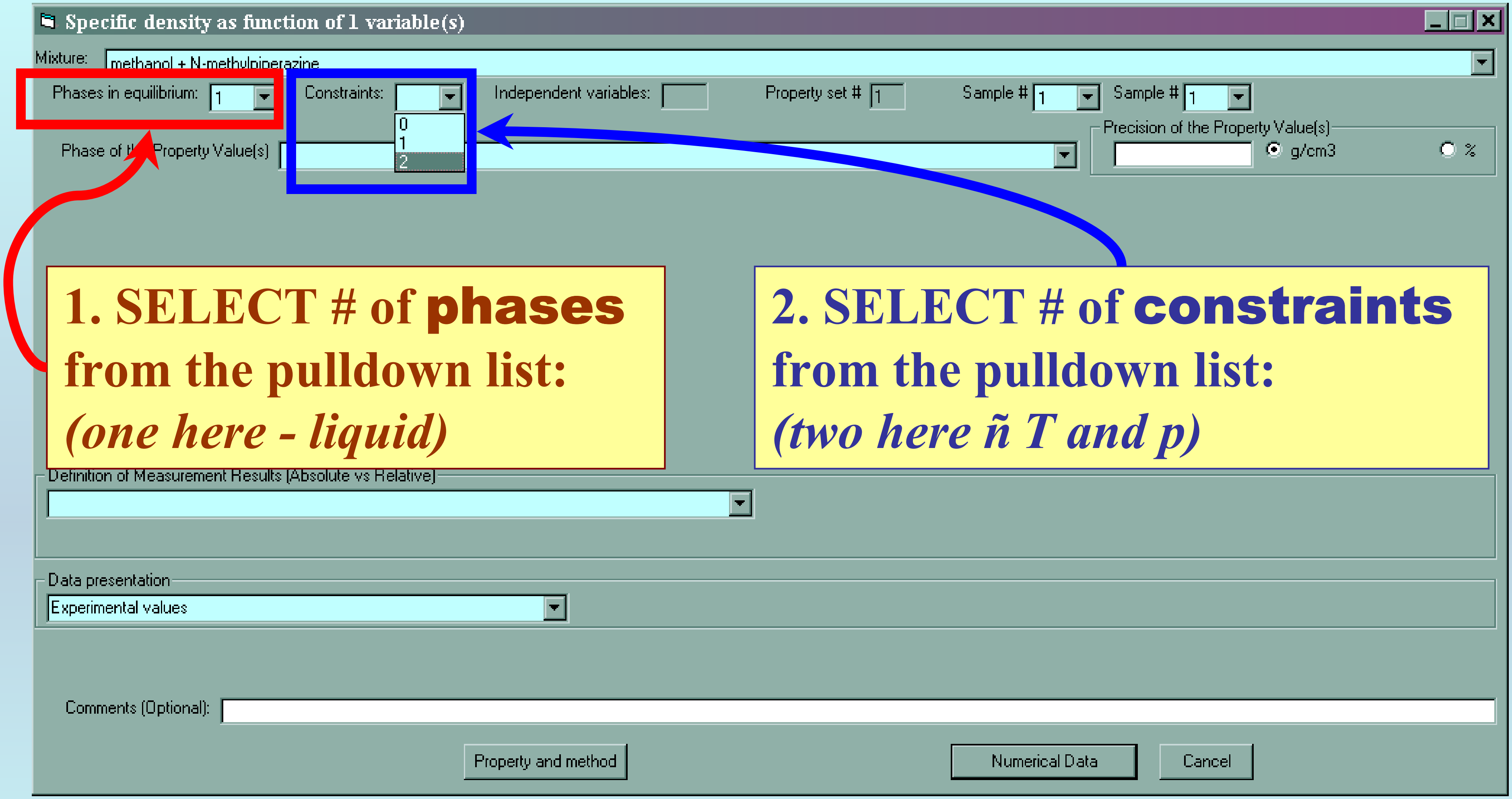
Experimental purpose: Principal objective of the work

Comment (optional):

Help
Details...
Table of values
Single value
Cancel

1. CLICK
Table of values

Specification of phases and constraints



Specific density as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1

Constraints: 0 / 1 / 2

Independent variables:

Property set # 1

Sample # 1

Sample # 1

Precision of the Property Value(s) ● g/cm3 ○ %

Phase of th Property Value(s)

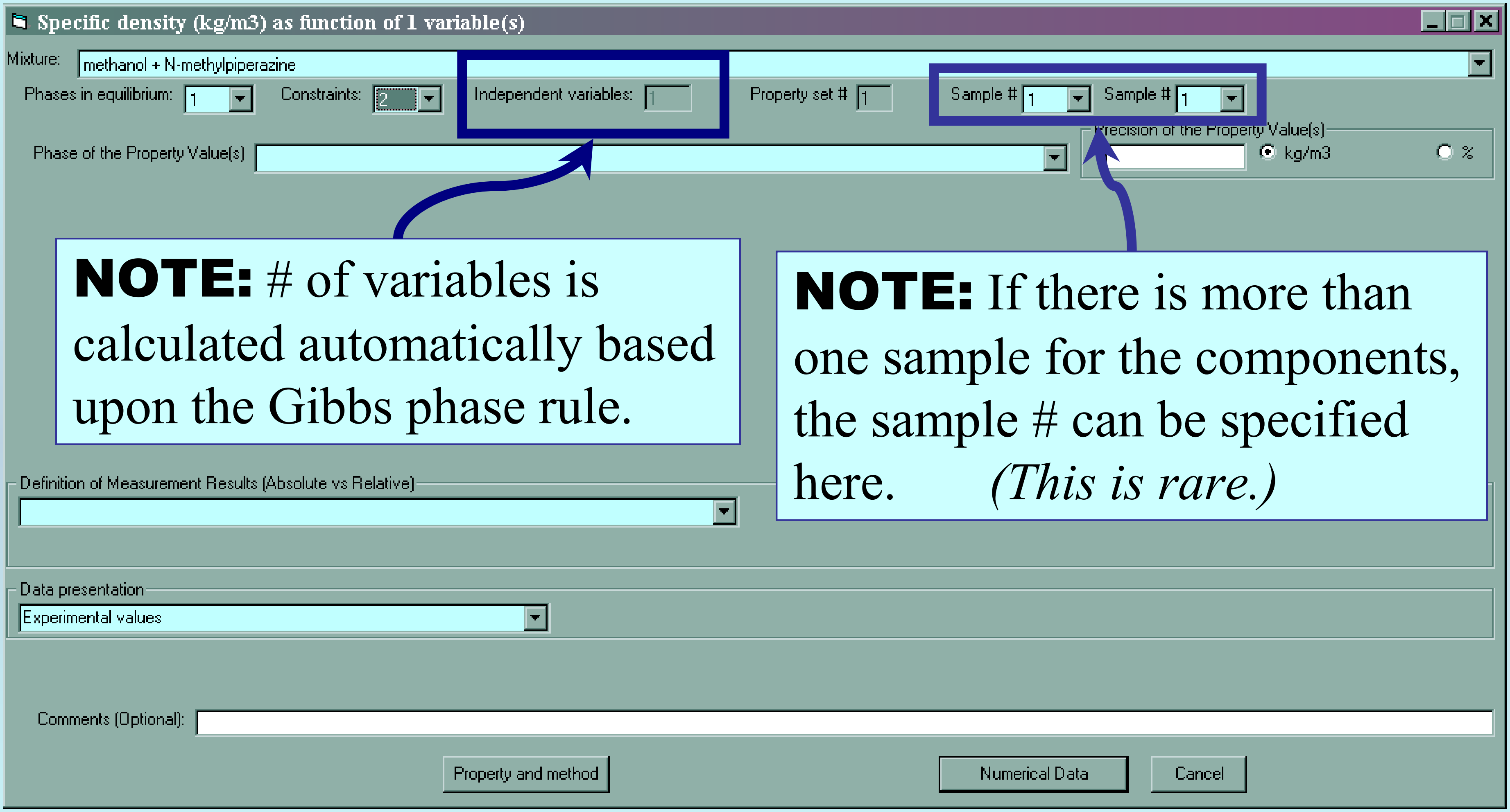
Definition of Measurement Results (Absolute vs Relative)

Data presentation: Experimental values

Comments (Optional):

1. SELECT # of **phases** from the pulldown list: *(one here - liquid)*

2. SELECT # of **constraints** from the pulldown list: *(two here ñ T and p)*



Specific density (kg/m3) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1

Constraints: 2

Independent variables: 1

Property set # 1

Sample # 1

Sample # 1

Phase of the Property Value(s)

Precision of the Property Value(s) ● kg/m3 ○ %

Definition of Measurement Results (Absolute vs Relative)

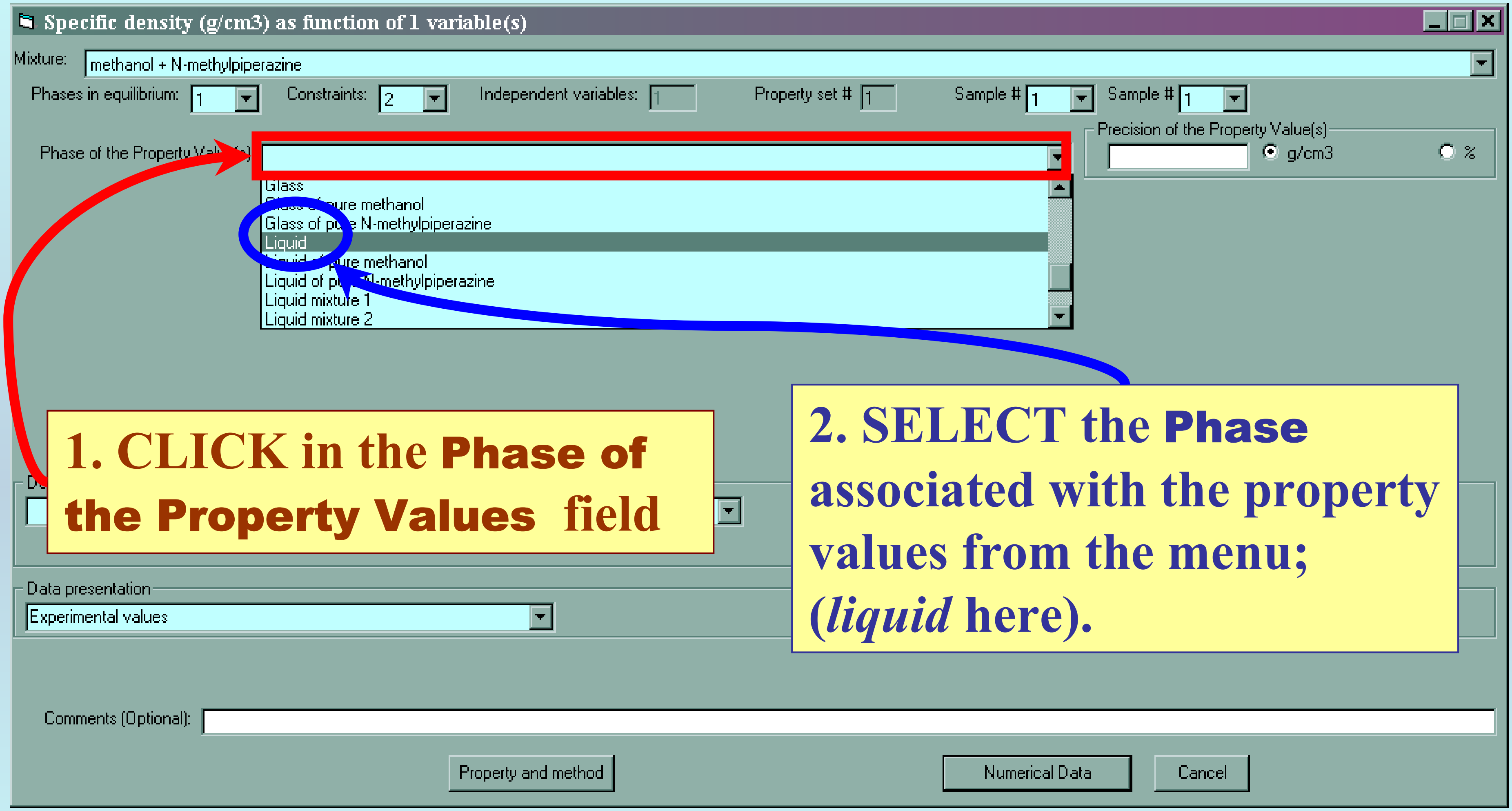
Data presentation: Experimental values

Comments (Optional):

NOTE: # of variables is calculated automatically based upon the Gibbs phase rule.

NOTE: If there is more than one sample for the components, the sample # can be specified here. *(This is rare.)*

Phase of the property value selection



Specific density (g/cm3) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1

Constraints: 2

Independent variables: 1

Property set # 1

Sample # 1

Sample # 1

Phase of the Property Value(s):

Precision of the Property Value(s): ● g/cm3 ○ %

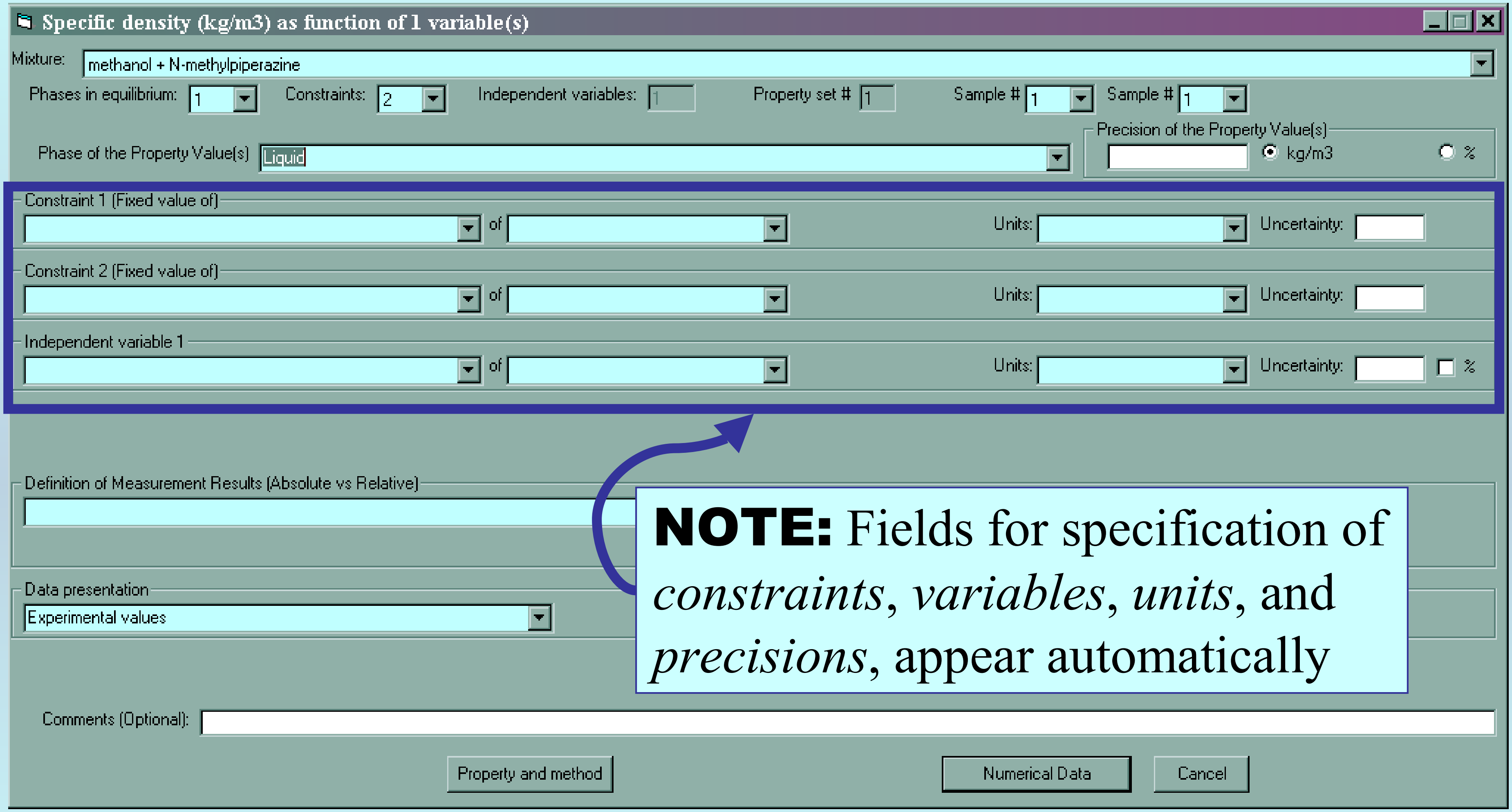
Data presentation: Experimental values

Comments (Optional):

Glass
Glass of pure methanol
Glass of pure N-methylpiperazine
Liquid
Liquid of pure methanol
Liquid of pure N-methylpiperazine
Liquid mixture 1
Liquid mixture 2
Property and method
Numerical Data
Cancel

1. CLICK in the **Phase of the Property Values** field

2. SELECT the **Phase** associated with the property values from the menu; (*liquid* here).


Constraint 1 (Fixed value of)
of
Units:
Uncertainty:
Constraint 2 (Fixed value of)
of
Units:
Uncertainty:
Independent variable 1
of
Units:
Uncertainty:
☐ %
Definition of Measurement Results (Absolute vs Relative)
Comments (Optional):
Property and method
Numerical Data
Cancel

Specific density (kg/m3) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1

Constraints: 2

Independent variables: 1

Property set # 1

Sample # 1

Sample # 1

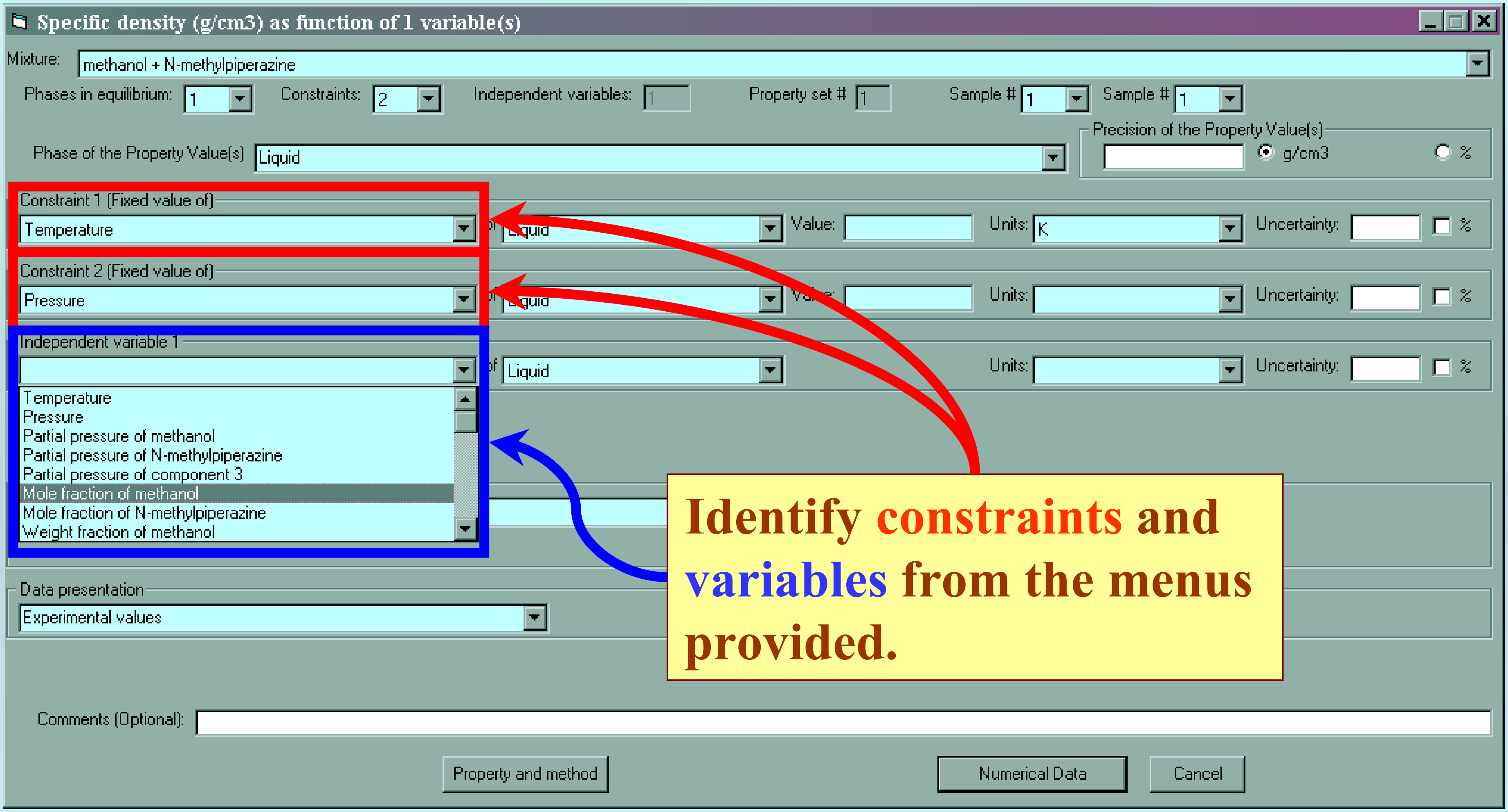
Phase of the Property Value(s) Liquid

Precision of the Property Value(s) ● kg/m3 ○ %

Data presentation: Experimental values

NOTE: Fields for specification of *constraints*, *variables*, *units*, and *precisions*, appear automatically

Variable and constraint identification



Specific density (g/cm3) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1

Constraints: 2

Independent variables: 1

Property set # 1

Sample # 1

Sample # 1

Phase of the Property Value(s): Liquid

Precision of the Property Value(s): ● g/cm3 ○ %

Constraint 1 (Fixed value of): Temperature; of: Liquid; Value: ; Units: K; Uncertainty: ; ☐ %

Constraint 2 (Fixed value of): Pressure; of: Liquid; Value: ; Units: ; Uncertainty: ; ☐ %

Independent variable 1: ; of: Liquid; Units: ; Uncertainty: ; ☐ %

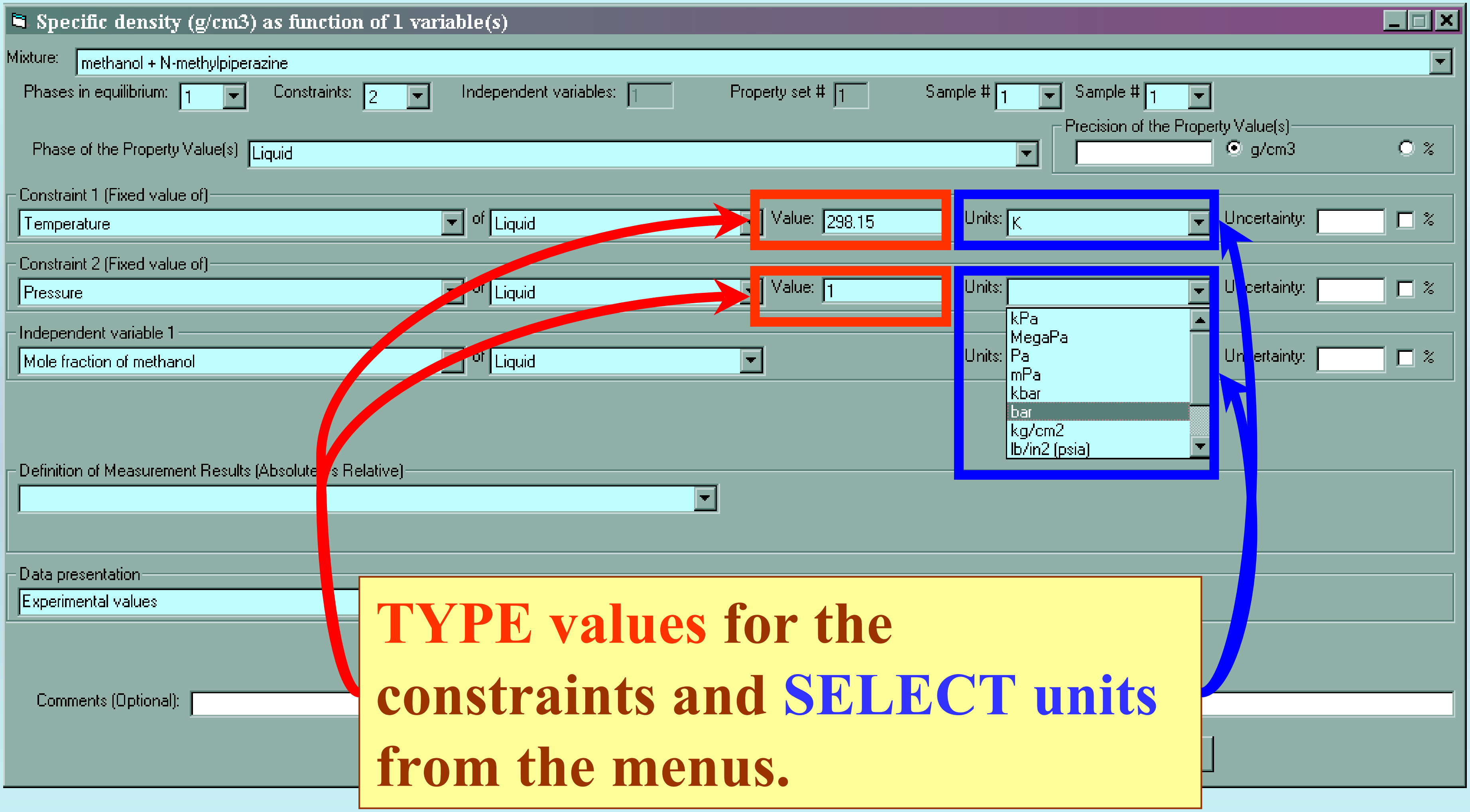
- Temperature
- Pressure
- Partial pressure of methanol
- Partial pressure of N-methylpiperazine
- Partial pressure of component 3
- Mole fraction of methanol
- Mole fraction of N-methylpiperazine
- Weight fraction of methanol

Data presentation: Experimental values

Comments (Optional):

Identify constraints and variables from the menus provided.

Entry of values for constraints



Specific density (g/cm3) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1
Constraints: 2
Independent variables: 1
Property set # 1
Sample # 1
Sample # 1

Phase of the Property Value(s) Liquid

Precision of the Property Value(s) ● g/cm3 ○ %

Constraint 1 (Fixed value of) Temperature of Liquid Value: 298.15 Units: K Uncertainty: ☐ %

Constraint 2 (Fixed value of) Pressure of Liquid Value: 1 Units: Uncertainty: ☐ %

Independent variable 1 Mole fraction of methanol of Liquid Units: Uncertainty: ☐ %

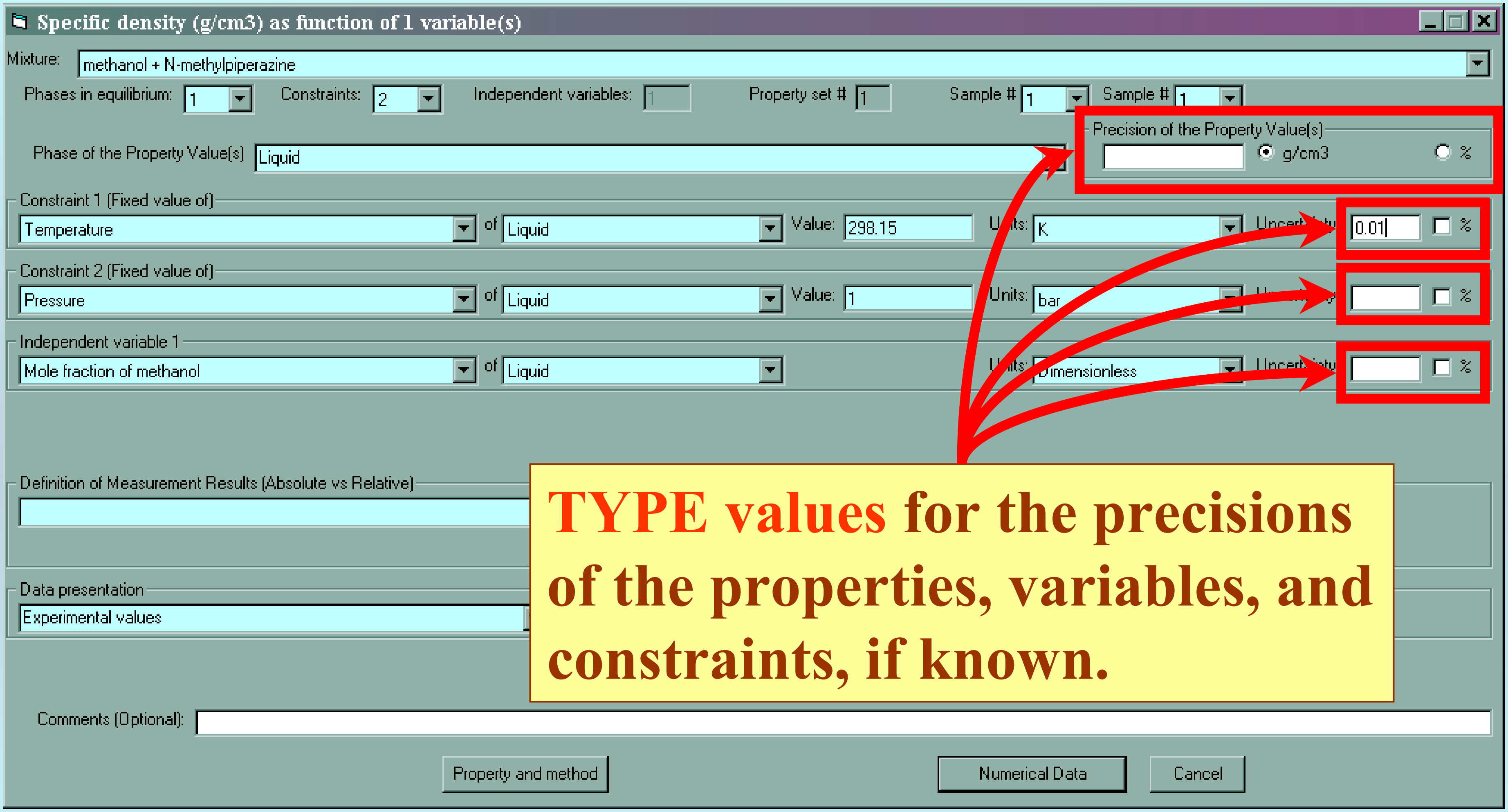
Definition of Measurement Results (Absolute vs Relative)

Data presentation Experimental values

Comments (Optional):

TYPE values for the constraints and SELECT units from the menus.

Capture of precisions, if known



Specific density (g/cm3) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1

Constraints: 2

Independent variables: 1

Property set # 1

Sample # 1

Sample # 1

Phase of the Property Value(s): Liquid

Precision of the Property Value(s): ● g/cm3 ○ %

Constraint 1 (Fixed value of): Temperature of Liquid; Value: 298.15; Units: K; 0.01 ☐ %

Constraint 2 (Fixed value of): Pressure of Liquid; Value: 1; Units: bar; ☐ %

Independent variable 1: Mole fraction of methanol of Liquid; Units: Dimensionless; ☐ %

Definition of Measurement Results (Absolute vs Relative)

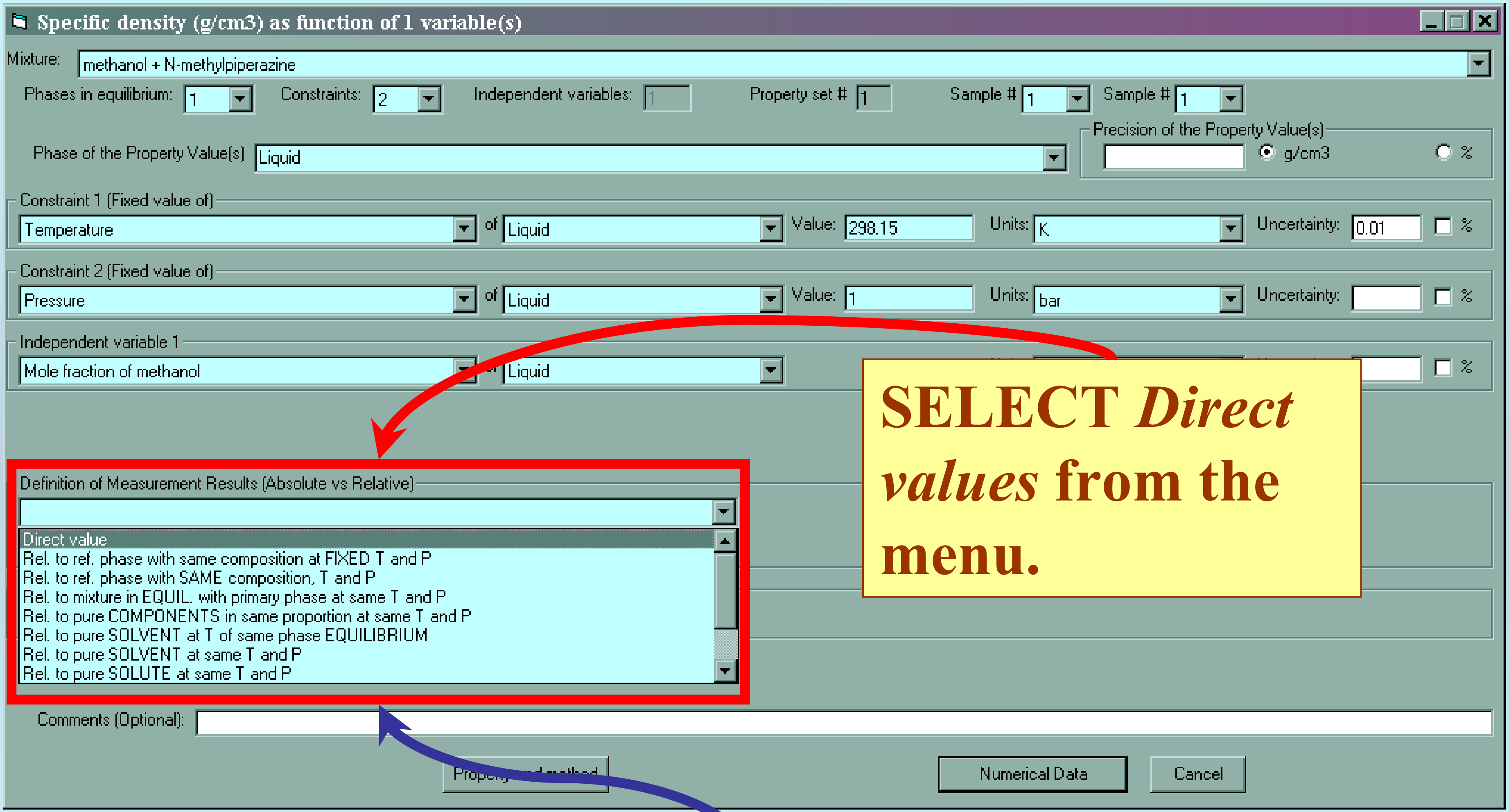
Data presentation: Experimental values

Comments (Optional):

TYPE values for the precisions of the properties, variables, and constraints, if known.

NOTE: Only the precision of temperature was provided by the authors in this example.

Define results: Absolute vs Relative



Specific density (g/cm3) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1
Constraints: 2
Independent variables: 1
Property set # 1
Sample # 1
Sample # 1

Phase of the Property Value(s) Liquid

Precision of the Property Value(s) ● g/cm3 ○ %

Constraint 1 (Fixed value of)
Temperature of Liquid Value: 298.15 Units: K Uncertainty: 0.01 ☐ %

Constraint 2 (Fixed value of)
Pressure of Liquid Value: 1 Units: bar Uncertainty: ☐ %

Independent variable 1
Mole fraction of methanol of Liquid ☐ %

Definition of Measurement Results (Absolute vs Relative)

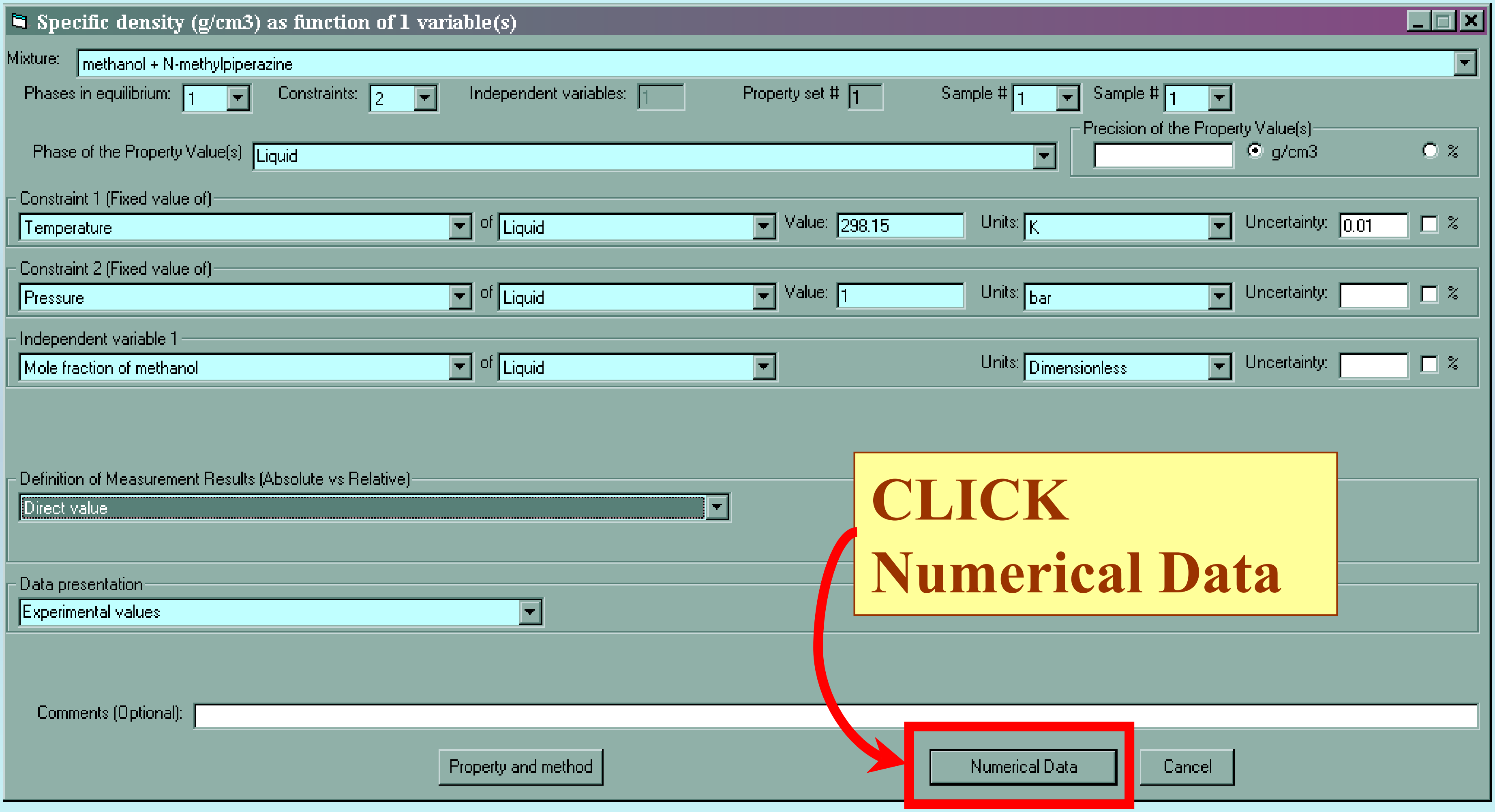
- Direct value
- Rel. to ref. phase with same composition at FIXED T and P
- Rel. to ref. phase with SAME composition, T and P
- Rel. to mixture in EQUIL. with primary phase at same T and P
- Rel. to pure COMPONENTS in same proportion at same T and P
- Rel. to pure SOLVENT at T of same phase EQUILIBRIUM
- Rel. to pure SOLVENT at same T and P
- Rel. to pure SOLUTE at same T and P

Comments (Optional):

SELECT *Direct values* from the menu.

NOTE: Other options are typically for data reported as relative values (e.g., relative to the density of the pure solovent). These are not common.

Form is complete...



Specific density (g/cm3) as function of 1 variable(s)

Mixture: methanol + N-methylpiperazine

Phases in equilibrium: 1

Constraints: 2

Independent variables: 1

Property set # 1

Sample # 1

Sample # 1

Phase of the Property Value(s) Liquid

Precision of the Property Value(s) ● g/cm3 ○ %

Constraint 1 (Fixed value of) Temperature of Liquid Value: 298.15 Units: K Uncertainty: 0.01 ☐ %

Constraint 2 (Fixed value of) Pressure of Liquid Value: 1 Units: bar Uncertainty: ☐ %

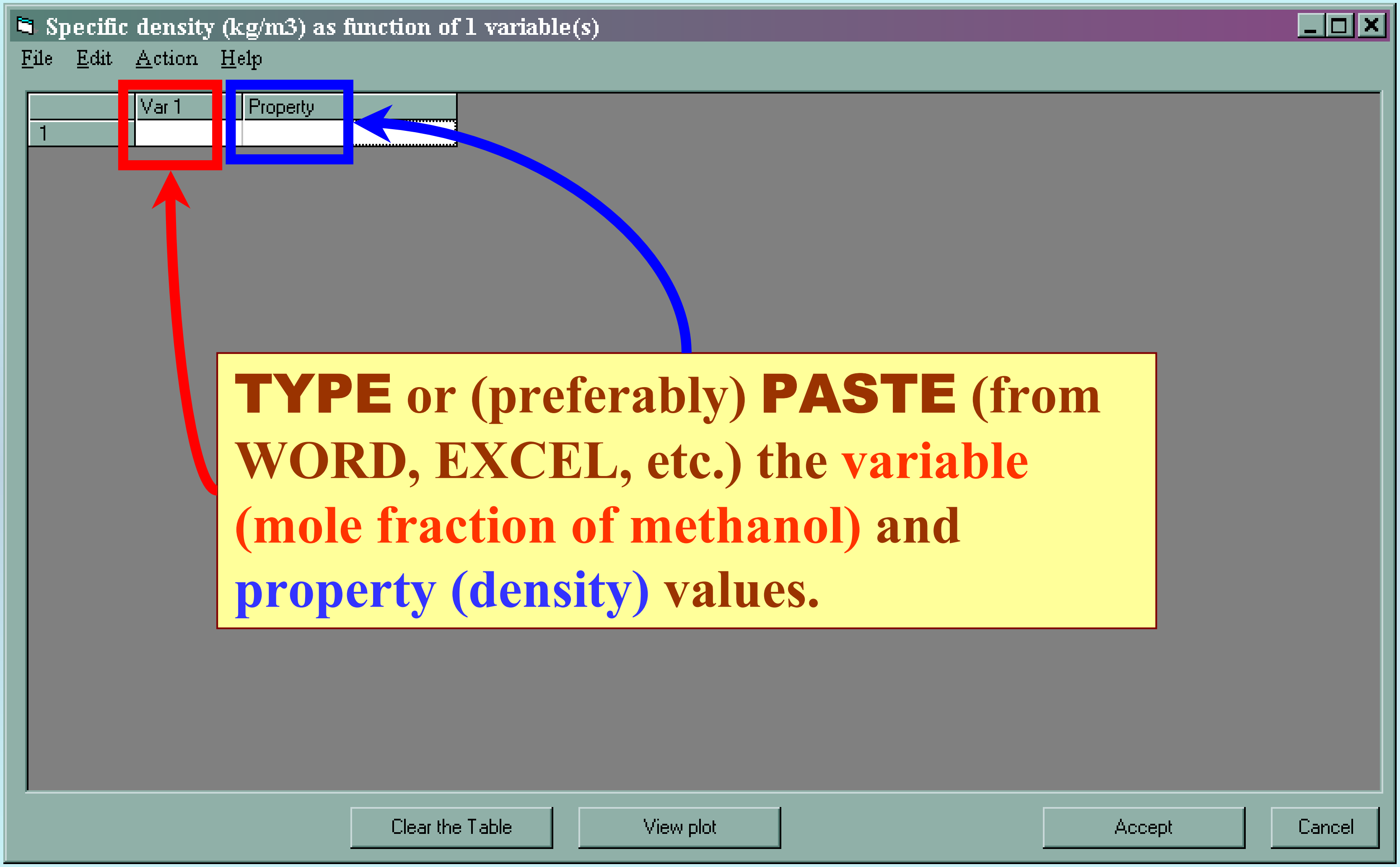
Independent variable 1 Mole fraction of methanol of Liquid Units: Dimensionless Uncertainty: ☐ %

Definition of Measurement Results (Absolute vs Relative) Direct value

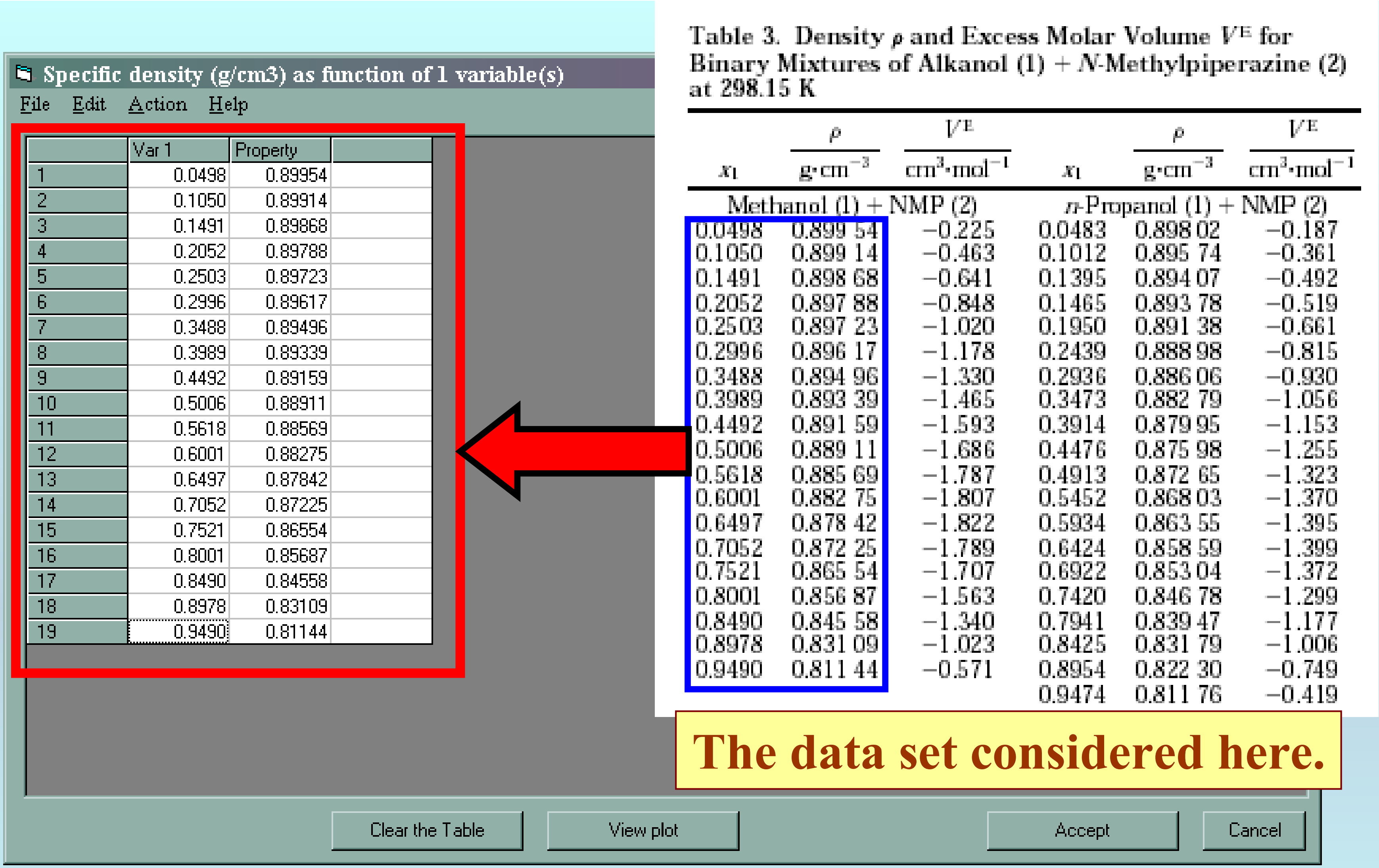
Data presentation Experimental values

Comments (Optional):

CLICK Numerical Data


Specific density (kg/m3) as function of 1 variable(s)
File
Edit
Action
Help
Var 1
Property
1
Clear the Table
View plot
Accept
Cancel

TYPE or (preferably) **PASTE** (from WORD, EXCEL, etc.) the variable (mole fraction of methanol) and property (density) values.



	Var 1	Property	
1	0.0498	0.89954	
2	0.1050	0.89914	
3	0.1491	0.89868	
4	0.2052	0.89788	
5	0.2503	0.89723	
6	0.2996	0.89617	
7	0.3488	0.89496	
8	0.3989	0.89339	
9	0.4492	0.89159	
10	0.5006	0.88911	
11	0.5618	0.88569	
12	0.6001	0.88275	
13	0.6497	0.87842	
14	0.7052	0.87225	
15	0.7521	0.86554	
16	0.8001	0.85687	
17	0.8490	0.84558	
18	0.8978	0.83109	
19	0.9490	0.81144	

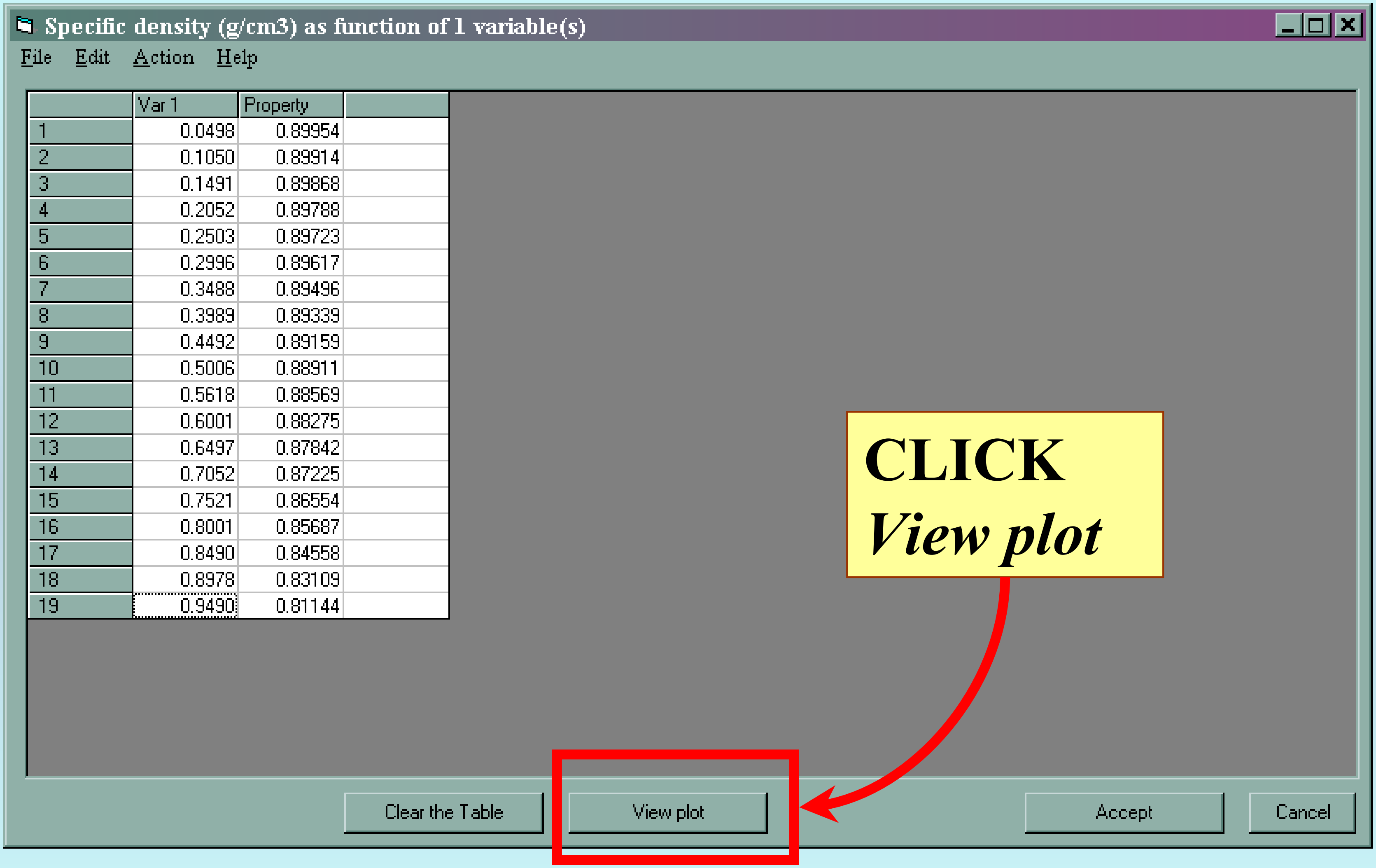
Table 3. Density ρ and Excess Molar Volume V^E for Binary Mixtures of Alkanol (1) + *N*-Methylpiperazine (2) at 298.15 K

x_1	ρ / $g \cdot cm^{-3}$	V^E / $cm^3 \cdot mol^{-1}$	x_1	ρ / $g \cdot cm^{-3}$	V^E / $cm^3 \cdot mol^{-1}$
Methanol (1) + NMP (2)			*n*-Propanol (1) + NMP (2)		
0.0498	0.899 54	−0.225	0.0483	0.898 02	−0.187
0.1050	0.899 14	−0.463	0.1012	0.895 74	−0.361
0.1491	0.898 68	−0.641	0.1395	0.894 07	−0.492
0.2052	0.897 88	−0.848	0.1465	0.893 78	−0.519
0.2503	0.897 23	−1.020	0.1950	0.891 38	−0.661
0.2996	0.896 17	−1.178	0.2439	0.888 98	−0.815
0.3488	0.894 96	−1.330	0.2936	0.886 06	−0.930
0.3989	0.893 39	−1.465	0.3473	0.882 79	−1.056
0.4492	0.891 59	−1.593	0.3914	0.879 95	−1.153
0.5006	0.889 11	−1.686	0.4476	0.875 98	−1.255
0.5618	0.885 69	−1.787	0.4913	0.872 65	−1.323
0.6001	0.882 75	−1.807	0.5452	0.868 03	−1.370
0.6497	0.878 42	−1.822	0.5934	0.863 55	−1.395
0.7052	0.872 25	−1.789	0.6424	0.858 59	−1.399
0.7521	0.865 54	−1.707	0.6922	0.853 04	−1.372
0.8001	0.856 87	−1.563	0.7420	0.846 78	−1.299
0.8490	0.845 58	−1.340	0.7941	0.839 47	−1.177
0.8978	0.831 09	−1.023	0.8425	0.831 79	−1.006
0.9490	0.811 44	−0.571	0.8954	0.822 30	−0.749
			0.9474	0.811 76	−0.419

The data set considered here.

Type **or (preferably)** ***Paste***
from WORD, EXCEL, etc.

Graphical check for typographical errors

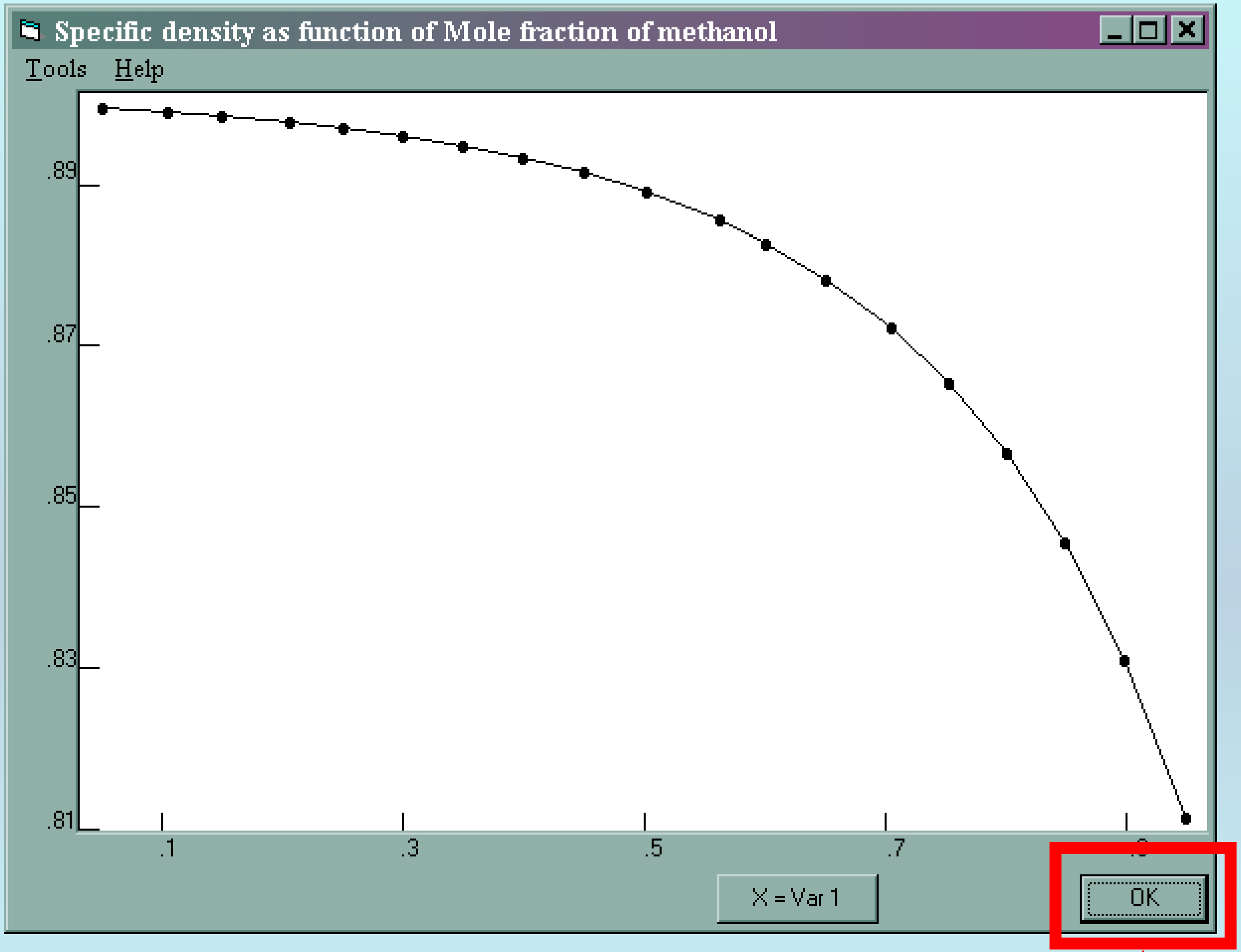

File
Edit
Action
Help
Clear the Table
View plot
Accept
Cancel

Specific density (g/cm3) as function of 1 variable(s)

	Var 1	Property	
1	0.0498	0.89954	
2	0.1050	0.89914	
3	0.1491	0.89868	
4	0.2052	0.89788	
5	0.2503	0.89723	
6	0.2996	0.89617	
7	0.3488	0.89496	
8	0.3989	0.89339	
9	0.4492	0.89159	
10	0.5006	0.88911	
11	0.5618	0.88569	
12	0.6001	0.88275	
13	0.6497	0.87842	
14	0.7052	0.87225	
15	0.7521	0.86554	
16	0.8001	0.85687	
17	0.8490	0.84558	
18	0.8978	0.83109	
19	0.9490	0.81144	

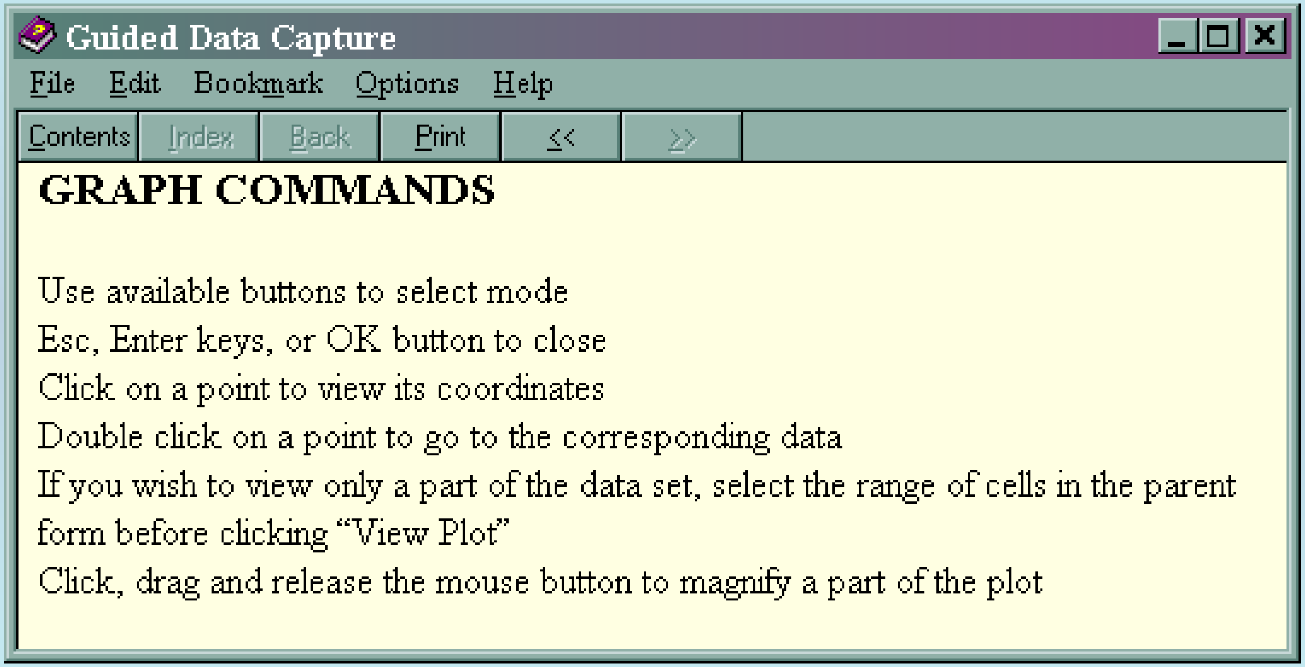
CLICK
View plot

Inspect plot


Specific density as function of Mole fraction of methanol
Tools
Help
.89
.87
.85
.83
.81
.1
.3
.5
.7
X = Var 1
OK

CLICK *OK*, if satisfied

NOTE: **The plots have several useful features. See the *HELP* screen on the plot.**


Guided Data Capture
File
Edit
Bookmark
Options
Help
Contents
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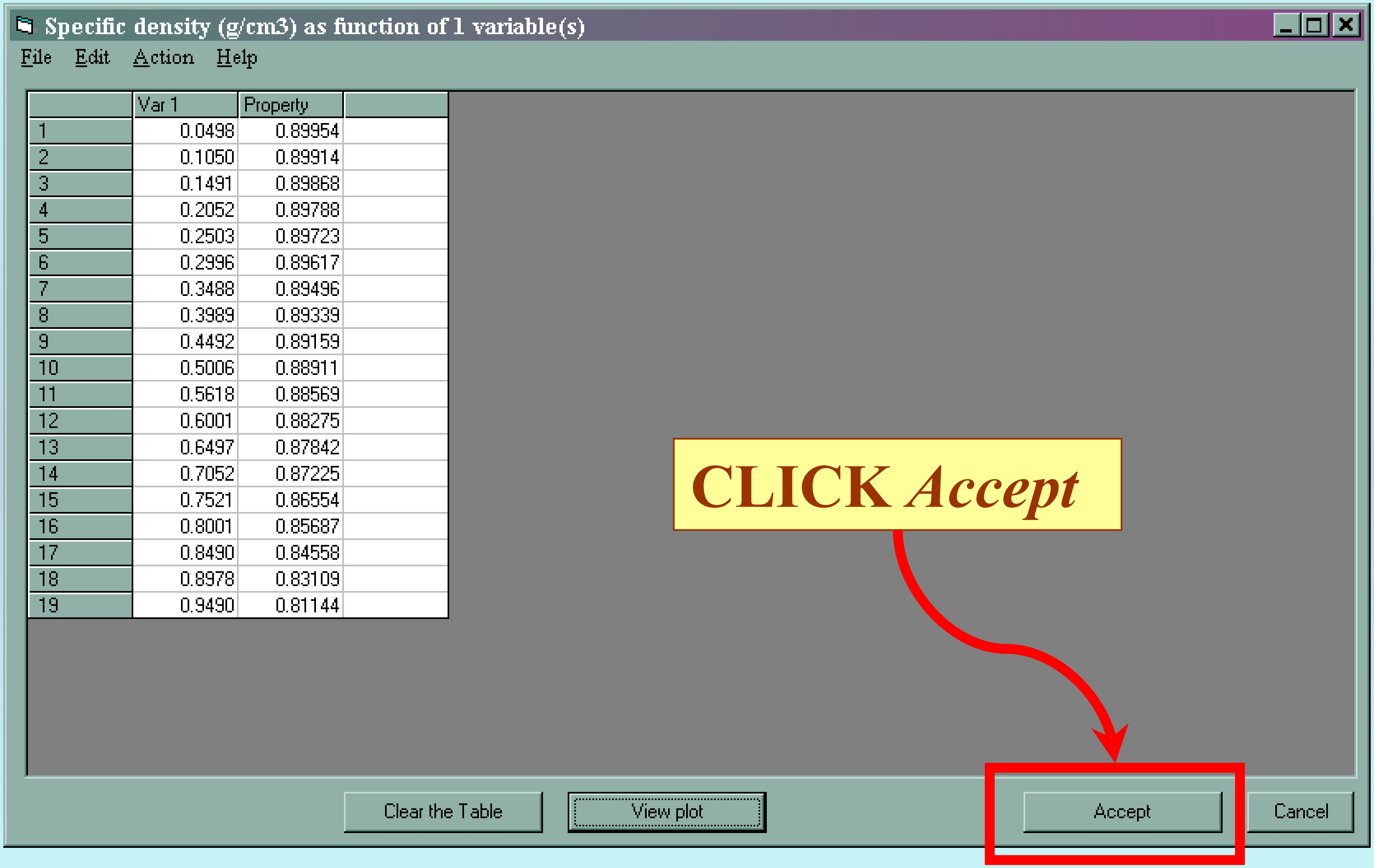
GRAPH COMMANDS

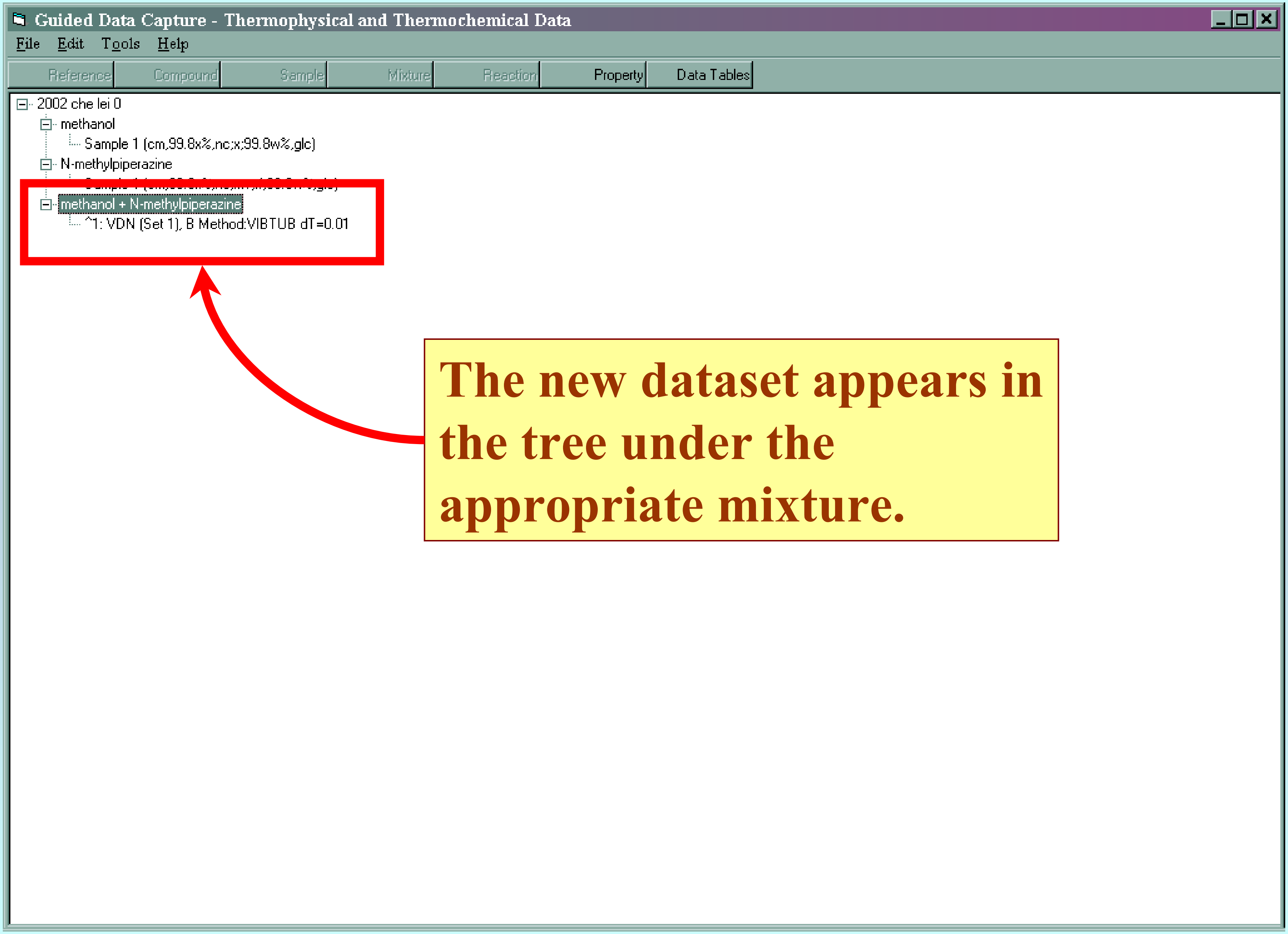
Use available buttons to select mode
Esc, Enter keys, or OK button to close
Click on a point to view its coordinates
Double click on a point to go to the corresponding data
If you wish to view only a part of the data set, select the range of cells in the parent form before clicking "View Plot"
Click, drag and release the mouse button to magnify a part of the plot

Final acceptance


Specific density (g/cm3) as function of 1 variable(s)
File
Edit
Action
Help
Clear the Table
View plot
Accept
Cancel

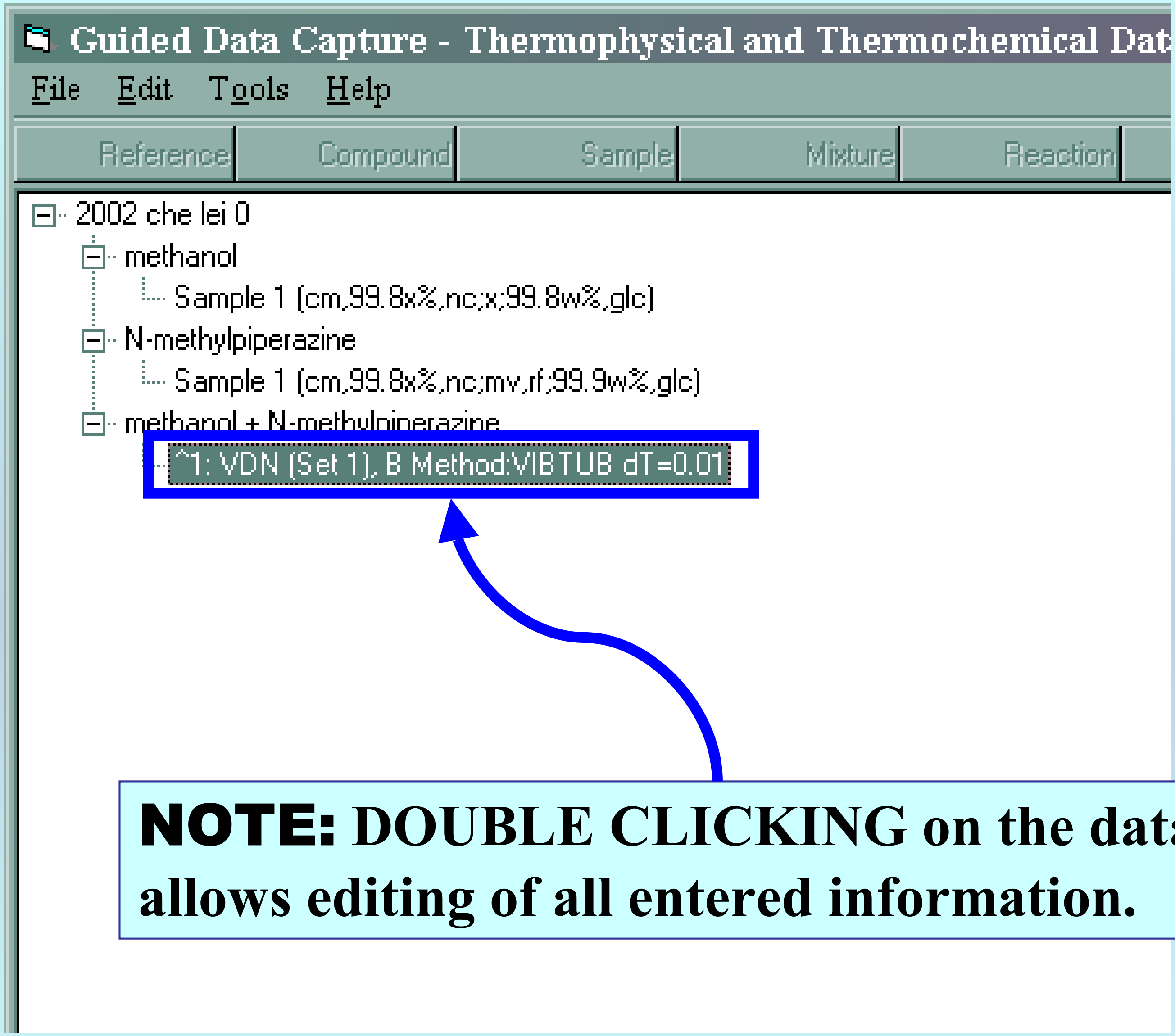
	Var 1	Property
1	0.0498	0.89954
2	0.1050	0.89914
3	0.1491	0.89868
4	0.2052	0.89788
5	0.2503	0.89723
6	0.2996	0.89617
7	0.3488	0.89496
8	0.3989	0.89339
9	0.4492	0.89159
10	0.5006	0.88911
11	0.5618	0.88569
12	0.6001	0.88275
13	0.6497	0.87842
14	0.7052	0.87225
15	0.7521	0.86554
16	0.8001	0.85687
17	0.8490	0.84558
18	0.8978	0.83109
19	0.9490	0.81144

CLICK *Accept*


Guided Data Capture - Thermophysical and Thermochemical Data
File
Edit
Tools
Help
Reference
Compound
Sample
Mixture
Reaction
Property
Data Tables

2002 che lei 0
  methanol
    Sample 1 (cm,99.8x%,nc;x;99.8w%,glc)
  N-methylpiperazine
    Sample 1 [illegible]
  methanol + N-methylpiperazine
    ^1: VDN (Set 1), B Method:VIBTUB dT=0.01

The new dataset appears in the tree under the appropriate mixture.


Guided Data Capture - Thermophysical and Thermochemical Dat
File
Edit
Tools
Help
Reference
Compound
Sample
Mixture
Reaction

2002 che lei 0
  methanol
    Sample 1 (cm,99.8x%,nc;x;99.8w%,glc)
  N-methylpiperazine
    Sample 1 (cm,99.8x%,nc;mv,rf;99.9w%,glc)
  methanol + N-methylpiperazine
    ^1: VDN (Set 1), B Method:VIBTUB dT=0.01

NOTE: **DOUBLE CLICKING on the dataset allows editing of all entered information.**

END

Continue with other compounds, samples, properties, reactions, etc...

or **save your file and exit the program.**